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SOME APPLICATIONS OF THE QUANTUM CELL MODEL

A THESIS

Presented to
The Faculty of the Graduate Division
by
Julio Fernando Fernández

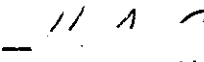
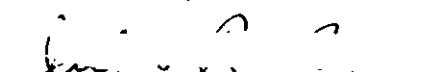

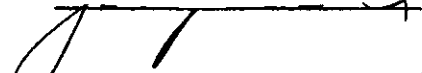
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CHAPTER I

INTRODUCTION

Experiments of Significance

The first well known experimental observation on the peculiar properties of helium four at very low temperatures was made by Kamerlingh Onnes¹ in 1911. He found that the thermal expansion coefficient became negative for temperatures below 2.2°K. Onnes and Boks² made more elaborate measurements in 1924, which disclosed a discontinuity in the thermal expansion coefficient. In 1928 Keesom and Wolfke,³ comparing the discontinuity to a phase transition were the first to use the terminology "helium I" and "helium II," helium II being the low temperature form. Specific heat measurements by Keesom and Clausius⁴ in 1932 showed a singularity of the specific heat curve in the shape of the letter λ ; thus the name λ transition. λ transitions are not first order phase transitions, that is, the entropy and volume remain constant at the transition.

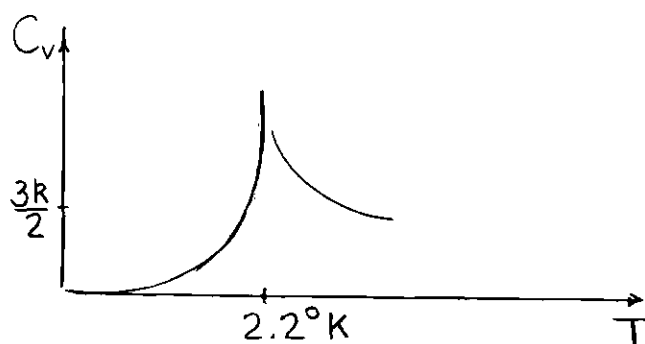


Figure 1. Experimental Specific Heat of Liquid He^4 Along the Vapor Pressure Curve.

Subsequent investigations established the melting curve and λ transition at different pressures as shown on Figure 2.

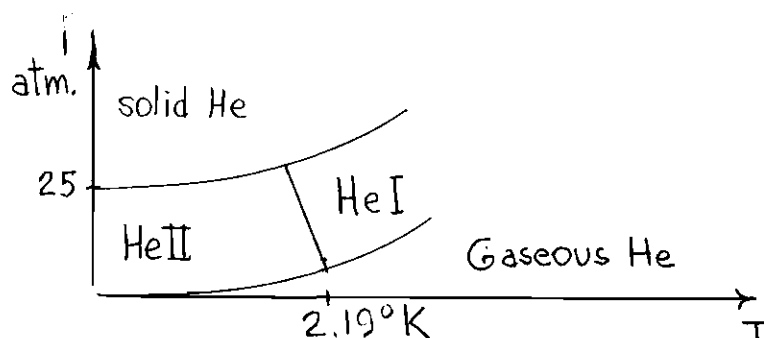


Figure 2. Phases of He^4 .

Along the solid fluid line the slope of pressure versus temperature goes to zero as $T \rightarrow 0$. This follows from the Clausius-Clapeyron equation

$$\frac{dp}{dT} = \frac{S_2 - S_1}{V_2 - V_1} \quad \text{and Nernst theorem.}$$

In 1930 Keesom and van den Ende⁵ observed accidentally that He II flowed easily through extremely small cracks which were tight for He I at higher temperatures. Thus, there appeared to be a large drop in viscosity in going from He I to He II. This was the first known evidence of the superfluid properties of He II.

Kapitza,⁶ and independently Allen and Neisener,⁷ repeated measurements based on the "capillary flow method" showing the viscosity of liquid helium dropping by many orders of magnitude to an immeasurably small value when the temperature was lowered through the λ point.

Another very interesting phenomenon was discovered by Allen and Jones⁸ in 1938. The apparatus used is shown in schematic form in Figure 3.

The apparatus consists of a reservoir and a small vessel connected by a capillary. In the experiment He II was used, and the level in the

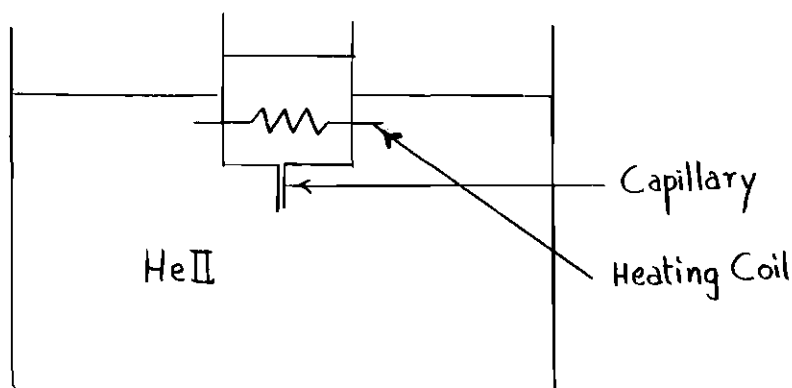


Figure 3. Schematic Diagram of the Fountain Effect.

vessel rose above the level in the reservoir when heat was applied.

By 1939 enough significant experiments had been performed for the beginnings of the development of a theory to explain the peculiar behavior of He II.

As it turned out, the most profitable characteristics of He II on which to focus attention were the specific heat curve, from $T = 0$ up to $T > T_\lambda$, and the superfluid properties.

One of the first models was proposed by Fröhlich⁹ in 1937. He tried to explain the λ transition as an order-disorder transition between n holes and n helium atoms in a $\frac{2n}{2}$ centered cubic lattice of places. This idea must have been induced by the fact that λ transitions of the order-disorder type occur in solid lattice. He treated the transition in analogy with the second order transition in B-brass. Closer analysis of the model, by London,¹⁰ showed that no such transition could occur. In the same paper London pointed out that in the Bose-Einstein condensation there is a discontinuity in the derivative of the specific heats at $T = 3.09^\circ\text{K}$ for a density equal to that of He^4 at zero pressure. The Bose-Einstein condensation is a transition of third order (discontinuity in the derivative of C_v whereas the He^4 λ transition appeared at

the time to be a transition of second order (discontinuity in the specific heat). London said in his paper "Though actually the λ -point of helium resembles a phase transition of second order, it seems difficult not to imagine a connection with the condensation phenomenon of the Bose-Einstein statistics." In this paper London was not proposing a model, but he was merely pointing out that Einstein condensation in a free particle system and the λ -transition in Helium four appeared to have a connection, or, to put it another way, they appeared to be basically the same type of phenomenon. This paper by London proved to be a guiding light in the search for a model and explanation from first principles of the peculiar properties of liquid helium II. It should be noticed that a system of free particles cannot show superfluid properties at any temperature because of the energy dependence on momentum. It will be shown later that an excitation of momentum p and energy $\epsilon = \frac{p^2}{2m}$ cannot exist in a superfluid. Thus, the ideal gas Einstein condensation gives the correct qualitative description of the specific heat, but it furnishes the incorrect qualitative properties of a superfluid. Tisza^{11,12,13,14} escaped the pitfalls of this molecular model while using the basic idea in it to postulate his microscopic model of helium II. The postulates as stated by Tisza¹⁴ are:

1. The ground state energy $E_0(N)$ has a minimum for some value $V = V_0$ of the volume:

$$\frac{\partial E_0}{\partial V} \bigg|_{V=V_0} = 0, \quad \frac{\partial^2 E_0}{\partial V^2} \bigg|_{V=V_0} > 0.$$

2. The state $E_0(V)$ is characterized by a vanishing microscopic rigidity.

3. The shear modes of motion of helium have a gaseous character. The "elementary excitations" correspond to translation of atoms (or group of atoms) with definite values of mass momentum and energy.

4. There exists a temperature T_0 such that:

$$\begin{aligned} &= 0 \quad \text{if } T = 0 && \text{He II} \\ \frac{\rho_n}{\rho} &< 1 \quad \text{if } 0 < T < T_0 && \text{He II} \\ &= 1 \quad \text{if } T \geq T_0 && \text{He I} \end{aligned}$$

with $\frac{\rho_n}{\rho}$ monotonically increasing between $T = 0$ and $T = T_0$. To be identified with the λ transition temperature E_0 is the ground state energy of the system. The first postulate is a statement of the fact that helium is not a gas at $T = 0$ i.e. there exists a $V = V_0$ for which $P = 0$. The second postulate states that helium is not a solid at $T = 0$, and furthermore its viscosity vanishes at that temperature. The third postulate states that the "elementary excitations" are *eigenvalues* of both momentum and energy and correspond to a mass motion. They interact with the walls of the vessel but not among each other, i.e. they behave as a very dilute gas.

The fourth postulate, the most important one, states that there is some mass in the ground state for $0 \leq T < T_0$, this mass decreasing monotonically as T increases from $T = 0$ to $T = T_0$, $\frac{\rho_n}{\rho}$ being the fraction of mass moving with the elementary excitations.

Thus there are two phases in the II, not separable in ordinary space, but separated in momentum space, the phase in zero momentum being superfluid while the normal phase shows viscous flow.

The fountain effect, previously mentioned, will now be explained

in terms of the model of Tisza. It will be remembered that two vessels were connected by a capillary thin enough to stop the flow of He I and He gas. The superfluid phase of He II can flow through the capillary. It follows from Nernst's theorem that the superfluid phase carries no entropy with it, therefore there will be no heat exchange among the two vessels if one assumes the walls to be thermally insulating. The system is, therefore, in mechanical equilibrium but not in thermal equilibrium.

If one has a system in mechanical as well as thermal equilibrium, then one can write from the second and first laws of thermodynamics the following relations:

$$\left(\frac{\partial S_1}{\partial E_1} \right)_{V_1} = \frac{1}{T_1} = \left(\frac{\partial S_2}{\partial E_2} \right)_{V_2} = \frac{1}{T_2}$$

$$\left(\frac{\partial S_1}{\partial V_1} \right)_{E_1} = P_1 = \left(\frac{\partial S_2}{\partial V_2} \right)_{E_2} = P_2$$

where the subscript 1 associates a quantity with the first vessel and the subscript 2 with the second one and $P_1 = P_2$; $T_1 = T_2$. However in the case under consideration the systems are not in thermal contact; therefore the entropy should not be maximized and P_1 need not equal P_2 , and T_1 need not equal T_2 . This is the crux of the matter. One vessel may thus have a higher pressure head than the other vessel and a different temperature also. The differences $T_2 - T_1$ and $P_2 - P_1$ are related as will be shown.

Since the entropy of the whole system is fixed and cannot be changed by any transfer of mass through the capillary, the condition to

be satisfied by the system is that the energy should be minimum.

The energy of each vessel is a function of the number of particles, the volume and the entropy. $E_1(N_1, V_1, S_1)$, $E_2(N_2, V_2, S_2)$ but S_1 and S_2 are fixed, so the condition is

$$\frac{\partial E_1}{\partial N_1} dN_1 + \frac{\partial E_2}{\partial N_2} dN_2 + \frac{\partial E_1}{\partial V_1} dV_1 + \frac{\partial E_2}{\partial V_2} dV_2 = 0.$$

So $\frac{\partial E_1}{\partial N_1} = \frac{\partial E_2}{\partial N_2}$ since $dN_1 = -dN_2$; on the other hand $dV_1 \neq dV_2$ in

general so $\frac{\partial E_1}{\partial V_1} \neq \frac{\partial E_2}{\partial V_2}$ in general, i.e. $\mu_1(P_1, T_1) = \mu_2(P_2, T_2)$ and

$P_1 \neq P_2$ in general. So the usual phase equilibrium relation for the chemical potential is obtained, but the pressures and temperatures do not need to be equal. One may now change T_1 and P_1 with no change in μ_1 , but one is allowed to keep P_2 and T_2 constant. Therefore assuming one starts from $T_1 = T_2$ and $P_1 = P_2$ one may have

$$\mu_1(T_1 + \Delta T, P_1 + \Delta P) = \mu_2(T_1, P_1)$$

and so

$$\frac{\partial \mu_1}{\partial T_1} \Delta T + \frac{\partial \mu_1}{\partial P_1} \Delta P = 0.$$

but

$$\frac{\partial \mu}{\partial T}_P = -S \quad \text{and} \quad \frac{\partial \mu}{\partial P}_T = \frac{1}{\rho}.$$

so:

$$\Delta P = \rho S \Delta T.$$

As a result one vessel may be under a pressure ΔP higher and ΔT temperature higher than the other vessel with ΔP and ΔT related by the last expression. Thus a vessel maintained at a higher temperature will be under a higher pressure head than the other vessel, and provided that their only connection is the capillary they will maintain the difference in pressure and temperature ad infinitum. Thinking in very crude terms what happens goes something like this: If one starts out with two vessels, one at temperature $T + \Delta T$ the other at temperature T and they both have equal mass, then the vessel at higher temperature will have less superfluid mass than the other vessel, according to Tisza's fourth postulate. If the two vessels are now connected by a capillary allowing only superfluid flow, then one would expect fluid to flow from the vessel with more superfluid mass (lower temperature) to the vessel with less superfluid mass (higher temperature) thus establishing a higher pressure head on the latter vessel. On the other hand, if one has two vessels with equal mass and same temperature and pressure connected by a capillary, and one applies a mechanical pressure to the first vessel some fluid should flow to the second vessel. Now the first vessel will contain a smaller fraction of superfluid than the second vessel, therefore it follows from Tisza's fourth postulate that the temperature of the first vessel increases. This is termed the mechanocaloric effect. It had not been observed at the time Tisza's proposed his model; this effect was found experimentally by Daunt and Mendelssohn¹⁵ in 1939.

The model proposed by Tisza had no justification from first principles. The main task in the superfluidity of helium problem after 1938 was the explanation of the properties of He II with a molecular

theory starting from first principles. The first step in this direction was taken by Landau^{7,8} when he postulated an energy spectrum for He II for energies slightly different from the ground state energy. The energy spectrum was postulated, not derived from first principles, and Landau advanced no argument to show why this energy spectrum, which guaranteed the superfluidity of He⁴ at low enough temperatures, should not apply in the case of He³ which does not show any superfluid property at any temperature so far obtained (at the time Landau wrote his first paper He³ had not been subject to experiments because it is rather rare, 1/1,200,000 is the ratio of He³ to He⁴ in atmospheric helium, as well as helium from wells). The first experiment with He³ at low temperatures was conducted in 1948 by Osborne, Weinstock and Abraham¹⁹ with He³ obtained in nuclear experiments. It was found that He³ showed a viscosity of the same order of magnitude as that of He⁴ above 2.19°K for temperatures as low as 1.05°K. In 1958 capillary flow measurements by Zinov'eva²⁰, at temperatures as low as 0.35°K showed no superfluid behavior in He³. Landau postulated an energy spectrum to obtain the correct temperature dependence of the specific heat at temperatures near zero degrees absolute. It will be remembered that $C_V \sim T^3$, for solids near zero degrees absolute. At that temperature the excitations are phonons in the solid. For He⁴ $C_V \sim T^3$ at T near zero in the liquid state, so Landau postulated phonons to be the thermal excitations in He⁴. This implies the superfluid properties of He II as it will be shown below.

Let U be the energy of the system, $\epsilon(k)$ the energy eigenvalues

$$U = \sum_i \frac{\epsilon_i g_i}{e^{\frac{\epsilon_i}{kT}} - 1} \quad \text{and } g_i \text{ the number of degenerate states.}$$

$$= \frac{V}{(2\pi)^3} \int \frac{\epsilon(k) 4\pi k^2 dk}{e^{\frac{\epsilon(k)}{kT}} - 1}$$

where V is the volume of the system. Landau let $\epsilon = \hbar c |k|$ for T near zero.

So $d\epsilon = \hbar c dk$ and $\epsilon^2 = \hbar^2 c^2 k^2$ then

$$U = \frac{V}{(2\pi)^3} \int \frac{4\pi \frac{\epsilon^2}{c^2} \epsilon \frac{d\epsilon}{c} \frac{1}{\hbar^3}}{e^{\frac{\epsilon}{kT}} - 1}$$

$$U \sim T^4$$

and $C_V \sim T^3$ as required.

The energy spectrum postulated by Landau is

$$\begin{aligned} \epsilon(k) &= \hbar c k \quad \text{for } k \ll k_0 \\ &= \Delta + \frac{\hbar^2 (k - k_0)^2}{2\sigma} \quad \text{for } k \approx k_0. \end{aligned}$$

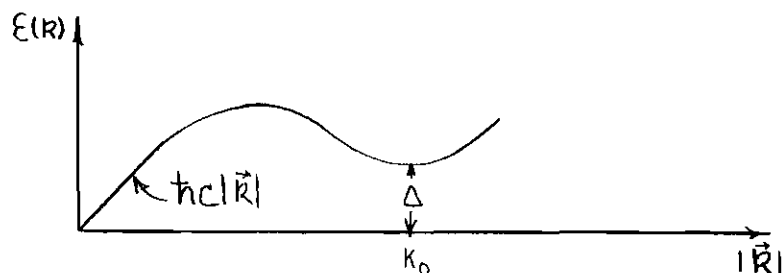


Figure 4. Landau's Energy Spectrum.

The following argument is taken from Landau²¹ to show how such an energy spectrum implies superfluidity.

Consider the liquid system in the ground state with the capillary walls moving with respect to it with velocity V . If there is some viscosity the liquid will eventually start moving. Motion can only appear after the excitation of interval motions i.e. appearance in the liquid of elementary excitation of momentum \bar{P} and energy $\epsilon(\bar{P})$. Then the energy of the liquid will be in its own coordinate system, $E_0 = \epsilon(\bar{P})$ and its momentum $\bar{P}_0 = \bar{P}$. By means of a Galilean transformation one may get the energy E of the liquid system in a coordinate system at rest with respect to the walls. Thus,

$$E = E_0 + \bar{P}_0 \cdot \bar{V}_1 + \frac{MV^2}{2}.$$

The term $\frac{MV^2}{2}$ represents the original energy of the liquid. $E_0 + \bar{P}_0 \cdot V$ must be negative since the energy of the moving system must decrease

$$\epsilon(\bar{P}) + \bar{P} \cdot \bar{V} < 0$$

$\epsilon(\bar{P}) + \bar{P} \cdot \bar{V}$ is a minimum when $\bar{P} \cdot \bar{V} = -|\bar{P}| |\bar{V}|$ i.e. the inequality can, at best, be satisfied if

$$v > \frac{\epsilon(\bar{P})}{|\bar{P}|}$$

but $\epsilon(P) = C|\bar{P}|$, so $V > C$ that is, no elementary excitation can appear so long as the velocity of the fluid with respect to the walls is less than the critical velocity C .

Thus, the energy spectrum postulated by Landau ensures the correct temperature dependence of the specific heat near $T = 0$, and gives the

desired superfluid behavior of the II. It must be remembered that this energy spectrum was postulated and not derived from first principles, and Landau gives no reason why such an energy spectrum should not be postulated for He^3 .

A significant contribution was made by Bogoljubov²² in 1947 when he showed by means of the operator formalism that a very dilute system of Bosons with weak interactions does have an energy spectrum of the type $\epsilon = C |\bar{P}|$ for low \bar{P} . Bogoljubov made the assumption that the fraction of particles with momentum different from zero was much less than one, thus limiting the velocity of his results to very dilute systems. He was the first one to show from first principles that there was a system of particles with the desired energy spectrum.

Feynman²³ was able to obtain, in 1954, Landau's energy spectrum by minimizing the energy. His results were not limited to dilute systems, but only limited to a system with small number of excitations. Feynman assumed a state function for the system to be $\Psi = \sum_{i=1}^N f(r_i) \phi$, ϕ being the ground state function. He showed that several other choices of Ψ gave a higher energy than the energy obtained from the postulated Ψ . He then minimized the energy using a variational technique to find $f(r_i) = \sum_{\vec{r}} e^{i\vec{k} \cdot \vec{r}_i}$.

One may not be satisfied with the fact that an a priori assumption was made about the form of Ψ .

An improvement on Bogoljubov's work was made by Lee,²⁴ Huang and Yang in 1957 by doing away with the limitation that the interaction should be weak. They treated a system of hard spheres with the method of pseudo-potentials and operator formalism. First they obtained the matrix elements

of the Hamiltonian considering only the interactions of particles with zero momentum, thus limiting the validity of their results to very dilute systems. They, then, diagonalized the Hamiltonian, thus obtaining the energy spectrum of the system. Again the energy spectrum was of the form $\epsilon = \hbar^2 |k|$ for low R and a small fraction of particles with momentum different from zero. Later, Huang considered a system of Bosons with weak attractions. Again, the results were only valid for low densities and the assumption was made that the fraction of particles with momentum different from zero was much less than one.

With the exception of Feynman's work, everyone of these papers is based on the assumption that $\frac{\sum n_k}{N} \ll 1$, where n_k is the average number of particles with momentum k . London¹⁵ remarked "... the central problem of the superfluid does not require the consideration of a whole canonical ensemble since the transition into the superfluid state can be performed at absolute zero by varying a macroscopic parameter, pressure, we actually have to deal with a pure mechanism involving a single quantum state, the ground state. Hence this is a problem of pure quantum mechanics." It was the purpose of the paper by Gersch²⁵ and Knollman to solve the problem as London suggests with no assumption regarding the average numbers of particles in the zero momentum state. The Green function technique was used in this problem decoupling the hierarchy of equations in a way that introduces no error in the limiting case of extremely high density.

A very brief sketch of the history of Green functions in statistical physics follows: the perturbation theory in statistical physics can lead to a series for the ground state energy in which the terms are proportional to powers of the volume. This terms must, of course, cancel

one another if one sums all the terms in the series. The Green function method, first used in quantum field theory, proved very useful in statistical physics. Expressions for the energy may be obtained with no higher powers of the volume. Also a decoupling of the hierarchy of Green functions equations may be related to certain physical assumptions about the system under consideration, thus establishing a region of validity for the results obtained. It allows a unified treatment of different many particle problems at $T = 0$ and $\rho \neq 0$.

One of the first to apply Green functions in statistical physics was Salam,³¹ in 1953, in rewriting Fröhlich's field theory of superconductivity. Spectral theorems for Green functions were considered by Bonch-Bruевич³² for $T = 0$ and by Landau³³ for $T \neq 0$. Green functions have been used in statistical mechanics by Gorkov³⁴ to obtain the energy spectrum of Bardeen,³⁵ Schrieffer, Cooper in the theory of superconductivity; by Beliaev^{36,37} to treat a dilute system of interacting Bosons; by Bogoljubov³⁸ and Tyablikov in the theory of ferromagnetism. These are but a few examples.

The Problem

It is the purpose of this investigation to extend the work done by Gersch²⁵ and Knollman by including attractive interactions in the Hamiltonian for a system of Bosons at $T = 0$ in the cell model; to apply the cell model Hamiltonian with short range repulsion to a system of Fermions, using Green functions at $T = 0$; and to treat a system of Bosons with short range repulsion, in the framework of the cell model, using Green functions at temperatures slightly different from zero.

Chapter II will deal with the formulation of the cell model.

In Chapter III a density for the solid fluid transition at $T = 0$ for Bosons with short range repulsive plus attractive interactions will be obtained.

In Chapter IV an improvement will be made on the approximation of Chapter III.

In Chapter V a system of Fermions with short range repulsive forces will be treated at $T = 0$ and extremely high densities.

Finally Chapter VI will deal with a system of Bosons with short range repulsive forces at $T \neq 0$. The specific heat will be obtained for the solid, a transition curve of ρ vs. T and a discussion of the superfluid in the cell model will be given. The Green function formalism to be used in this chapter is taken from a paper by Zubarev.⁴⁰

CHAPTER II

THE QUANTUM BELL MODEL

A system of spinless non-relativistic Bose particles in a large box is considered. The limit $N \rightarrow \infty$ and $\Omega \rightarrow \infty$ taken keeping $\frac{N}{\Omega}$ finite. The Hamiltonian for the system is

$$H = \frac{\hbar^2}{2m} \int \nabla \Psi^*(r) \cdot \nabla \Psi(r) d\tau + \frac{1}{2} \int \Psi^*(r) \Psi^*(r') U(r-r') \Psi(r') \Psi(r) d\tau d\tau' \quad (1)$$

where $\Psi^*(r)$ and $\Psi(r)$ are the creation and destruction operators of a particle at point r in the second quantization formalism. $U(r-r')$ is the two body potential interaction. The first term in the Hamiltonian is the kinetic energy operator and the second term is the potential energy operator. The operator for the total number of particles is given by

$$N = \int \Psi^*(r) \Psi(r) d\tau \quad (2)$$

$\Psi^*(r)$ and $\Psi(r)$ satisfy the usual commutation relations

$$\begin{aligned} [\Psi(r), \Psi(r')]_- &= [\Psi^*(r), \Psi^*(r')]_- = 0 \\ [\Psi(r), \Psi^*(r')]_- &= \delta(r - r') \end{aligned} \quad (3)$$

The central problem in this investigation will be the study of systems in the solid state at very low temperature at $T = 0$, as the density is lowered. The Green function technique will be used. The particle interactions cannot be treated as a perturbing term in describing

a system in the solid state. The two-particle Green functions cannot be approximated by a product of two one-particle Green functions; therefore one will have to solve a coupled set of integral differential equations to obtain the one particle Green function. To circumvent this difficulty the cell model will be introduced, as was done by Gersch²⁵ and Knochman. The field operators $\Psi^*(r)$ and $\Psi(r)$ are usually expanded using a complete set of functions:

$$\Psi(r) = \rho^{\frac{1}{2}} \sum_{r_j} b_{r_j} f(r - r_j) \quad (4)$$

If one uses an orthogonal, but incomplete, set of functions such as:

$$f(r - r_j) = \delta_{rr_j} = \begin{cases} 1 & \text{if } r \text{ is in cell centered on } r_j \\ 0 & \text{otherwise} \end{cases} \quad (5)$$

one will obtain a correct expansion of any function $\phi(r)$ in terms of this proposed set of functions as $\frac{\partial^2 \phi(r)}{\partial x^2} \rightarrow 0$ i.e. for infinite wave lengths. In more physical terms, one can never expect to obtain a good description of the motion of particles within their cells, or for excitations of the system with a large value of the momentum with this set of functions.

Close to the solid-superfluid transition, which is the region of primary interest here, the important momentum values are much smaller than \hbar times the inverse cell dimension, so that one can feel justified in the use of the cell model approximation.

The field operator $\Psi(r)$ has now the form

$$\Psi(r) = \rho^{\frac{1}{2}} \sum_{r_j} b_{r_j} \delta_{rr_j} \quad (6)$$

where $\rho = \frac{N}{\Omega}$; Ω being the volume of the system and N the total number of particles.

Multiplying (6) by $\delta_{r'r_k}$ and integrating over space one obtains

$$\int \Psi(r) \delta_{r'r_k} d\tau = \rho^{1/2} b_{r_k} \Delta V$$

where ΔV is the volume of one cell.

Similarly

$$\int \Psi^*(r) \delta_{r'r_k} d\tau = \rho^{1/2} b_{r_k}^* \Delta V$$

Now one may compute $[b_{r_i}, b_{r_j}^*]_-$

$$\begin{aligned} [b_{r_j}, b_{r_j}^*]_- &= \frac{1}{(\Delta V)^2} \int [\Psi(r), \Psi^*(r')]_- \delta_{rr_i} \delta_{r'r_j} \delta\tau d\tau' \\ &= \frac{1}{(\Delta V)^2} \Delta V \delta_{r_j r_j} \\ b_{r_j} b_{r_j}^* &= \frac{V}{N\Delta V} \delta_{r_j r_j} \end{aligned} \quad (8)$$

If the volume of the cells ΔV , is now chosen to be $\frac{V}{N}$, the specific volume, then b_{r_i} and $b_{r_i}^*$ are the destruction and creation operators of a particle in cell i .

Similarly, one finds:

$$[b_{r_j}, b_{r_k}]_- = [b_{r_j}^*, b_{r_k}^*]_- = 0 \quad (9)$$

Substituting $\psi(r)$ and $\psi^*(r)$ from equation (6) into equation (2) one obtains

$$N = \sum_{r_j} b_{r_j}^* b_{r_j} = \sum_{r_j} n_{r_j} \quad (10)$$

Using equation (6) the Hamiltonian of equation (1) will be expressed in terms of b_{r_j} and $b_{r_j}^*$ as follows:

$$\begin{aligned} H = & -\frac{\hbar^2}{2m} \int \rho^{\frac{1}{2}} \sum_{r_j} b_{r_j}^* \delta_{rr_j} \sum_{r_k} \rho^{\frac{1}{2}} b_{r_k} \nabla^2 \delta_{rr_k} d\tau \\ & + \frac{1}{2} \rho^2 \int \sum_{r_i} b_{r_i}^* \sum_{r_j} b_{r_j} U(r-r') \sum_{r_j} b_{r_k} \sum_{r_e} b_{r_e} \delta_{rr_i} \delta_{r'r_j} \delta_{r'r_k} \delta_{r'r_e} d\tau d\tau' \end{aligned} \quad (11)$$

Making use of the following finite approximation:

$$\nabla^2 \delta_{rr_j} \approx \frac{1}{r_0^2} \sum_{r_0} (\delta_{r, r_j+r_0} - 6\delta_{r, r_j}) \quad (12)$$

one obtains for the kinetic energy operator T :

$$T = \frac{\hbar^2 \rho^{2/3}}{2m} \left(6 \sum_{r_j} b_{r_j}^* b_{r_j} - \sum_{r_j r_0} b_{r_j}^* b_{r_j+r_0} \right) \quad (13)$$

where $r_0^3 = \frac{1}{\rho}$.

It is clear that the first term in the kinetic energy operator will yield the kinetic energy of localization of the particles to their cells. The expectation value of the second term will be different from zero if

the particles wander out of their cells. Particle wanderings decrease the kinetic energy as one would expect.

The second term in the Hamiltonian, the potential energy V , in equation (11), reduces to:

$$V = \frac{1}{2} \rho^2 \sum_{r_j} \sum_{r_k} b_{r_j}^* b_{r_k}^* b_{r_k} b_{r_j} \int_{\substack{r \text{ in cell } r_j \\ r' \text{ in cell } r_k}} U(r-r') d\tau d\tau' \quad (14)$$

Let

$$U_o = \rho \int_{\substack{r \text{ in cell } r_j \\ r' \text{ in cell } r_j}} U(r-r') d\tau d\tau'$$

and

$$U_{j_k} = \rho \int_{\substack{r \text{ in cell } r_j \\ r \text{ in cell } r_k}} U(r-r') d\tau d\tau' \quad j \neq k \quad (15)$$

Equation (14) can now be rewritten as:

$$V = \frac{1}{2} \rho \sum_{r_j} b_{r_j}^* b_{r_j}^* b_{r_j} b_{r_j} U_o + \frac{1}{2} \rho \sum_{r_j \neq r_k} b_{r_j}^* b_{r_k}^* b_{r_k} b_{r_j} U_{j_k} \quad (16)$$

Now

$$\begin{aligned} b_{r_j}^* b_{r_j}^* b_{r_j} b_{r_j} &= b_{r_j}^* (b_{r_j} b_{r_j}^* - 1) b_{r_j} \\ &= n_{r_j} n_{r_j} - n_{r_j} \end{aligned}$$

and

$$b_{r_j}^* b_{r_k}^* b_{r_k} b_{r_j} = b_{r_j}^* b_{r_j} b_{r_k}^* b_{r_k} \quad \text{with } r_j \neq r_k$$

$$= n_{r_j} n_{r_k}$$

Equation (16) may now be written as:

$$V = \frac{1}{2} \rho \sum_{r_j} (N_{r_j}^2 - N_{r_j}) U_0 + \frac{1}{2} \rho \sum_{r_j} \sum_{r_k} n_{r_j} n_{r_k} U_{j_k} \quad (17)$$

Finally, the Hamiltonian may be expressed as:

$$H = \frac{\hbar^2 \rho^{2/3}}{2m} \left(6 \sum_{r_j} b_{r_j}^* b_{r_j} - \sum_{r_j, r_0} b_{r_j}^* b_{r_j+r_0} \right) + \frac{\rho}{2} \sum_{r_j} b_{r_j}^* b_{r_j}^* b_{r_j} b_{r_j} U_0$$

$$+ \frac{\rho}{2} \sum_{r_j, r_k} b_{r_j}^* b_{r_k}^* b_{r_k} b_{r_j} U_{j_k} \quad (18)$$

or equivalently

$$H = \frac{\hbar^2 \rho^{2/3}}{2m} \left(6 \sum_{r_j} N_{r_j} - \sum_{r_j, r_0} b_{r_j}^* b_{r_j+r_0} \right) + \frac{\rho}{2} \sum_{r_j} (n_{r_j}^2 - n_{r_j}) U_0$$

$$+ \frac{\rho}{2} \sum_{r_j, r_k} n_{r_j} n_{r_k} U_{j_k}$$

It is illustrative to consider very briefly the very special case of a Dirac delta function type of interaction. Set $U(r-r') = c \delta(r-r')$, then $U_0 = c$ and $U_{j_k} = 0$. For a large enough value of ρ the potential energy term will be dominant in the Hamiltonian. One way to treat this

problem would be to find the eigenstates of the operator

$$6 \frac{\hbar^2 \rho^{2/3}}{2m} \sum_{r_j} n_{r_j} + \frac{\rho}{2} U_0 \sum_{r_j} (n_{r_j}^2 - n_{r_j}),$$

the ground state of this Hamiltonian would have one particle in each cell with no wanderings, and then treat

$$\frac{\hbar^2 \rho^{2/3}}{m} \sum_{r_j r_0} b_{r_j}^+ b_{r_j+r_0}$$

as a perturbation. It is clear, then, that as the value of ρ decreases the effect of the perturbing term will increase, and consequently the particle wanderings will increase. The term $\sum_{r_j r_0} b_{r_j}^* b_{r_j+r_0}$ will not be diagonal in the representation for which n_{r_j} is diagonal. This term will, from now on, be referred to as the off-diagonal term. Any approximations used for the off-diagonal term will be asymptotically exact as $\rho \rightarrow \infty$. These approximations will, of course, become worse as ρ decreases. Physically, one would expect these approximations to afford a good description of a system in its solid state, where the particle wanderings are very limited.

A system of non relativistic Bose particles with short range repulsion and nearest neighbor attractions will be treated in Chapters III and IV, i.e. $U_{j_k} = 0$ unless $\bar{r}_j - \bar{r}_k = \bar{r}_0$, $U_{j_k} < 0$ for $\bar{r}_j - \bar{r}_k = \bar{r}_0$.

A system of non relativistic Fermi particles will be treated in Chapter V with short range repulsive interactions, i.e. $U_{j_k} = 0$.

A system of non relativistic Bose particles with short range repulsive interactions, i.e. $U_{j_k} = 0$, at $T \neq 0$, will be treated in Chapter VI.

CHAPTER III

BOSONS WITH ATTRACTIVE INTERACTIONS AT $T = 0$

A system of non-relativistic, many Bose particles with short range repulsive and nearest neighbor attractive interactions at $T = 0$, i.e. $U_0 > 0$, $U_{jk} = 0$ for $\bar{r}_j \neq \bar{r}_k + \bar{r}_0$, $U_{jk} < 0$ for $\bar{r}_j = \bar{r}_k + \bar{r}_0$, and the system is in its ground state, will be considered in this and the next chapter.

The system will be observed as the pressure decreases from a very high value to zero, i.e. p decreases from a very high value to the value of p for which

$$\frac{\partial \langle \phi_0 | H(p) | \phi_0 \rangle}{\partial V} = 0$$

where $|\phi_0\rangle$ is the ground state vector function of the system. The value of p , $p(p = 0)$, for which

$$\frac{\partial \langle \phi_0 | H(p) | \phi_0 \rangle}{\partial V} = 0$$

will depend on U_{jk} , i.e. on the strength of the attractive interaction. The density of the solid fluid transition ρ_m , if there is one, will be obtained. If $\rho_m > \rho(p = 0)$ the system undergoes a transition, otherwise it does not. As shown in Chapter II the Hamiltonian of the system is given by:

$$\begin{aligned}
H = & 6K \sum_{r_j} b_{r_j}^* b_{r_j} - K \sum_{r_j, r_o} b_{r_j}^* b_{r_j+r_o} + \frac{1}{2} \rho \sum_{r_j} b_{r_j}^* b_{r_j}^* b_{r_j} b_{r_j} U_o + \\
& + \frac{1}{2} \rho \sum_{r_j, r_o} b_{r_j}^* b_{r_j} b_{r_j+r_o}^* b_{r_j+r_o} U_{r_j, r_j+r_o}
\end{aligned} \quad (3.1)$$

where

$$K = \frac{\hbar^2 \rho^{2/3}}{2m} \quad \text{let } U_{r_j, r_j+r_o} = \tilde{U} \quad (3.2)$$

The one-particle Green function furnishes, as is well known, the energy spectrum of a system. It is of great interest here to find out how the energy spectrum changes with the density of the system. In this way a density of transition will be obtained as well as the energy spectrum at the transition density. For this purpose the one-particle Green function is introduced now.

Let

$$G_1(j, k; t) = -i \langle \phi_o | T b_{r_j}(t) b_{r_k}^*(0) | \phi_o \rangle \quad (3.3)$$

where T is the usual Dyson chronological operator

$$\begin{aligned}
\langle \phi_o | T b_{r_j}(t) b_{r_k}^*(0) | \phi_o \rangle = & \theta(t) \langle \phi_o | b_{r_j}(t) b_{r_k}^*(0) | \phi_o \rangle + \\
& \theta(-t) \langle \phi_o | b_{r_j}(t) b_{r_k}^*(0) | \phi_o \rangle
\end{aligned}$$

G_1 is the usual causal Green function for Bosons. The dynamical equation of G_1 is given by:

$$\begin{aligned}
i \frac{\partial}{\partial t} G_1(j, k; t) &= i \left[\frac{\partial}{\partial t} - i \theta(t) \right] \langle \varphi_0 | b_{r_j}(t) b_{r_k}^+(0) | \varphi_0 \rangle + i \left[\frac{\partial}{\partial t} - i \theta(-t) \right] \langle \varphi_0 | b_{r_k}(0) \cdot \\
&\quad b_{r_j}^*(t) | \varphi_0 \rangle \\
&= \left[\frac{\partial}{\partial t} \theta(t) \right] \langle \varphi_0 | b_{r_j}(t) b_{r_k}^*(0) | \varphi_0 \rangle + \left[\frac{\partial}{\partial t} \theta(-t) \right] \cdot \\
&\quad \langle \varphi_0 | b_{r_k}^*(0) b_{r_j}(t) | \varphi_0 \rangle + \theta(t) \langle \varphi_0 | \frac{\partial}{\partial t} b_{r_j}(t) b_{r_k}(0) | \varphi_0 \rangle \\
&\quad + \theta(-t) \langle \varphi_0 | b_{r_k}^*(0) \frac{\partial}{\partial t} b_{r_j}(t) | \varphi_0 \rangle \quad (3.4)
\end{aligned}$$

but

$$\frac{\partial}{\partial t} \theta(t) = \delta(t) ; \quad \frac{\partial}{\partial t} \theta(-t) = -\delta(t) \quad (3.5)$$

and

$$-\frac{\partial b_{r_j}(t)}{\partial t} = \frac{1}{i} [b_{r_j}, H]_- \quad \text{with } \hbar = 1 \quad (3.6)$$

Now, from equation (3.1) one has

$$\begin{aligned}
[b_{r_j}, H]_- &= 6K \sum_{r_k} [b_{r_j}, b_{r_k}^* b_{r_k}] - K \sum_{r_k r_o} [b_{r_j}, b_{r_k}^* b_{r_k+r_o}]_- + \quad (3.7) \\
&+ \frac{1}{2} \rho U_o \sum_{r_k} [b_{r_j}, b_{r_k}^* b_{r_k}^* b_{r_k} b_{r_k}]_- + \\
&+ \frac{1}{2} \rho \tilde{U} \sum_{r_k r_o} [b_{r_j}, b_{r_k}^* b_{r_k} b_{r_k}^* b_{r_k+r_o} b_{r_k+r_o}]
\end{aligned}$$

The commutation relations given in equations (8) have to be used to obtain

$[b_{r_j}, H]_-$. This is done in Appendix A.

From equation (A.6) in the Appendix:

$$\begin{aligned}
 [b_{r_j}(t), H]_- = & 6K b_{r_j}(t) - K \sum_{r_0} b_{r_j+r_0}(t) + \frac{2}{2} \rho U_0 b_{r_j}^*(t) b_{r_j}(t) b_{r_j}(t) + \\
 & + \rho \tilde{U} \sum_{r_0} b_{r_j}(t) b_{r_j+r_0}^*(t) b_{r_j+r_0}(t) \quad (3.8)
 \end{aligned}$$

Substituting equations (3.5) and (3.8) into equation (3.4) and simplifying one obtains:

$$\begin{aligned}
 i \frac{\partial}{\partial t} G_1(j, k; t) = & \delta(t) \langle \varphi_0 | b_{r_j}(t) b_{r_k}^*(0) | \varphi_0 \rangle - \langle \varphi_0 | b_k^*(0) b_{r_j}(t) | \varphi_0 \rangle - \\
 & - i 6K \langle \varphi_0 | T b_{r_j}(t) b_{r_k}^*(0) | \varphi_0 \rangle + iK \langle \varphi_0 | T b_{r_j+r_0}(t) \\
 & b_{r_k}^*(0) | \varphi_0 \rangle - i \rho U_0 \langle \varphi_0 | T b_{r_j}^*(t) b_{r_j}(t) b_{r_j}(t) b_{r_k}^*(0) | \varphi_0 \rangle \\
 & - i \rho \tilde{U} \sum_{r_0} \langle \varphi_0 | T b_{r_j+r_0}^*(t) b_{r_j+r_0}(t) b_{r_j}(t) b_k^*(0) | \varphi_0 \rangle \quad (3.9)
 \end{aligned}$$

Let

$$G_2(j, k; t) = -i \langle \varphi_0 | T b_{r_j}^*(t) b_{r_j}(t) b_{r_j}(t) b_{r_k}^*(0) | \varphi_0 \rangle \quad (3.10)$$

It is necessary to obtain a dynamical equation of G_2 in order to solve (3.9). The equation of motion of G_2 is:

$$\begin{aligned}
 i \frac{\partial}{\partial t} G_2(j, k; t) = & \delta(t) \langle \varphi_0 | b_{r_j}^*(t) b_{r_j}(t) b_{r_j}(t) b_{r_k}^*(0) | \varphi_0 \rangle - \\
 & - \langle \varphi_0 | b_{r_k}^*(0) b_{r_j}^*(t) b_{r_j}(t) b_{r_j}(t) | \varphi_0 \rangle + \\
 & + \frac{1}{i} \langle \varphi_0 | T [b_{r_j}^*(t) b_{r_j}(t) b_{r_j}(t), H] b_{r_k}^*(0) | \varphi_0 \rangle \quad (3.11)
 \end{aligned}$$

From equation (A.11), in the Appendix:

$$\begin{aligned}
 b_{r_j}^*(t)b_{r_j}(t)b_{r_j}(t), H = & 6K b_{r_j}^*(t)b_{r_j}(t)b_{r_j}(t) \\
 & - 2K \sum_{r_0} b_{r_j}^*(t)b_{r_j}(t)b_{r_j+r_0}(t) + K \sum_{r_0} b_{r_j+r_0}^*(t)b_{r_j}(t)b_{r_j}(t) \\
 & + \rho U_0 b_{r_j}^*(t)b_{r_j}(t)b_{r_j}(t) + \rho U_0 b_{r_j}^*(t)b_{r_j}^*(t)b_{r_j}(t)b_{r_j}(t)b_{r_j}(t) + \\
 & + \rho \tilde{U} \sum_{r_0} b_{r_j}^*(t)b_{r_j}(t)b_{r_j}(t)b_{r_j+r_0}^*b_{r_j+r_0} \quad (3.12)
 \end{aligned}$$

One may now write the equation of motion of $G_2(j,k;t)$ as follows:

$$\begin{aligned}
 i \frac{\partial}{\partial t} G_2(j,k;t) = & 2b(t) \delta_{r_j,r_k} + 6K G_2(j,k;t) - \\
 & - 2K \sum_{r_0} (-i) \langle \varphi_0 | T b_{r_j}^*(t)b_{r_j}(t)b_{r_j+r_0}(t)b_{r_k}^*(0) | \varphi_0 \rangle + \\
 & + K \sum_{r_0} (-i) \langle \varphi_0 | T b_{r_j+r_0}^*(t)b_{r_j}(t)b_{r_j}(t)b_{r_k}^*(0) | \varphi_0 \rangle + \rho U_0 G_2(j,k;t) - \\
 & - i\rho U_0 \langle \varphi_0 | T b_{r_j}^*(t)b_{r_j}^*(t)b_{r_j}(t)b_{r_j}(t)b_{r_j}(t)b_{r_k}^*(0) | \varphi_0 \rangle - \\
 & - i\rho \tilde{U} \sum_{r_0} \langle \varphi_0 | T b_{r_j}^*(t)b_{r_j}(t)b_{r_j}(t)b_{r_j+r_0}^*(t)b_{r_j+r_0}(t)b_{r_k}(0) | \varphi_0 \rangle \quad (3.13)
 \end{aligned}$$

A termination of these equations will now be performed such that they will still describe the system under consideration with small error in the case of small fluctuations, i.e. $n^2 - n$ not too different from zero.

The following approximations are appropriate:

$$\begin{aligned}
\langle \varphi_0 | T b_{r_j}^* (t) b_{r_j} (t) b_{r_j} (t) b_{r_j+r_0}^* (t) b_{r_j+r_0} (t) b_{r_k}^* (0) | \varphi_0 \rangle &= \\
&= \langle \varphi_0 | T b_{r_j}^* b_{r_j} b_{r_j} b_{r_k}^* (0) | \varphi_0 \rangle \langle \varphi_0 | b_{r_j+r_0}^* b_{r_j+r_0} | \varphi_0 \rangle \quad (3.14)
\end{aligned}$$

$$\langle \varphi_0 | T b_{r_j}^* (t) b_{r_j}^* (t) b_{r_j} (t) b_{r_j} (t) b_{r_j} (t) b_{r_k}^* (0) | \varphi_0 \rangle = 0 \quad (3.15)$$

$$\begin{aligned}
\langle \varphi_0 | T b_{r_j}^* (t) b_{r_j} (t) b_{r_j+r_0} (t) b_{r_k}^* (0) | \varphi_0 \rangle &= \\
&= \langle \varphi_0 | b_{r_j}^* b_{r_j} | \varphi_0 \rangle \langle \varphi_0 | T b_{r_j+r_0} (t) b_{r_k}^* (0) | \varphi_0 \rangle \quad (3.16)
\end{aligned}$$

$$\begin{aligned}
\sum_{r_0} \langle \varphi_0 | T b_{r_j+r_0}^* (t) b_{r_j} (t) b_{r_j} (t) b_{r_k}^* (0) | \varphi_0 \rangle &= \\
&= \langle \varphi_0 | T b_{r_j} (t) b_{r_k}^* (0) | \varphi_0 \rangle \langle \varphi_0 | b_{r_j+r_0}^* b_{r_j} | \varphi_0 \rangle \quad (3.17)
\end{aligned}$$

$$\begin{aligned}
\langle \varphi_0 | T b_{r_j+r_0}^* (t) b_{r_j+r_0} (t) b_{r_j} (t) b_{r_k}^* (0) | \varphi_0 \rangle &= \\
&= \langle \varphi_0 | b_{r_j+r_0}^* b_{r_j+r_0} | \varphi_0 \rangle \langle \varphi_0 | T b_{r_j} (t) b_{r_k}^* (0) | \varphi_0 \rangle \quad (3.18)
\end{aligned}$$

These approximations are exact in the limit as $n^2 - n \rightarrow 0$, i.p.

as $\rho \rightarrow \infty$. Consider equation (3.14) for example,

$$\begin{aligned}
\langle \varphi_0 | T b_{r_j}^* (t) b_{r_j} (t) b_{r_j} (t) b_{r_j+r_0}^* (t) b_{r_j+r_0} (t) b_{r_k}^* (0) | \varphi_0 \rangle &= \\
&= \begin{cases} \langle \varphi_0 | b_{r_j}^* b_{r_j} b_{r_j} b_{r_j+r_0}^* b_{r_j+r_0} b_{r_k}^* (0) | \varphi_0 \rangle & \text{for } t > 0 \\ \langle \varphi_0 | b_{r_k}^* (0) b_{r_j}^* b_{r_j} b_{r_j} b_{r_j+r_0}^* b_{r_j+r_0} | \varphi_0 \rangle & \text{for } t < 0 \end{cases}
\end{aligned}$$

Now $\langle n_{r_j} \rangle = 1$ and for $\rho \rightarrow \infty$, i.e. $\langle n^2 - n \rangle = 0$, clearly

$$\begin{aligned} \langle \varphi_0 | b_{r_k}^* (0) b_{r_j}^* b_{r_j} b_{r_j} b_{r_j+r_0}^* b_{r_j+r_0} | \varphi_0 \rangle &= \\ &= \langle \varphi_0 | b_{r_k}^* (0) b_{r_j}^* b_{r_j} b_{r_j} | \varphi_0 \rangle \langle \varphi_0 | b_{r_j+r_0}^* b_{r_j+r_0} | \varphi_0 \rangle \end{aligned}$$

and since $[b_{r_j}^* b_{r_j} b_{r_j}, b_{r_j+r_0}^*, b_{r_j+r_0}]_- = 0$

one has

$$\begin{aligned} \langle \varphi_0 | b_{r_j}^* b_{r_j} b_{r_j} b_{r_j+r_0}^* b_{r_j+r_0} b_{r_k}^* (0) | \varphi_0 \rangle &= \\ &= \langle \varphi_0 | b_{r_j+r_0}^* b_{r_j+r_0} | \varphi_0 \rangle \langle \varphi_0 | b_{r_j}^* b_{r_j} b_{r_j} b_{r_k}^* (0) | \varphi_0 \rangle \end{aligned}$$

This is the approximation of equation (3.14). The spirit of the approximation in equation (3.15) is easy to see. The approximation of equation (3.16) is of the same type as the one in equation (3.14). The same is true of equations (3.17) and (3.18).

These approximations are not unique. There are different approximations which satisfy the requirement that they become asymptotically exact as $\rho \rightarrow \infty$. For example, one could write in place of equation (3.16) the following:

$$\begin{aligned} \langle \varphi_0 | T b_{r_j}^* (t) b_{r_j} (t) b_{r_j+r_0} (t) b_{r_k}^* (0) | \varphi_0 \rangle &\simeq \\ &\simeq \langle \varphi_0 | b_{r_j}^* b_{r_j} | \varphi_0 \rangle \langle \varphi_0 | T b_{r_j+r_0} (t) b_{r_k}^* (0) | \varphi_0 \rangle + \\ &+ \langle \varphi_0 | b_{r_j}^* b_{r_j+r_0} | \varphi_0 \rangle \langle \varphi_0 | T b_{r_j} (t) b_{r_k}^* (0) | \varphi_0 \rangle \end{aligned}$$

Such approximation was considered for the simple case of $\tilde{U} = 0$. The use of this approximation yielded an energy which did not agree with a perturbation calculation of the energy to first order in $\frac{K}{\rho U_0}$. It would be an endless job to consider every different possible approximation. One can only say that the approximations used here do satisfy the requirement imposed on them, and they furnish sensible results.

The approximated equations for $G_1(j,k;t)$ and $G_2(j,k;t)$ (equations 3.9 and 3.13) now appear as:

$$\begin{aligned} (i \frac{\partial}{\partial t} - 6K - 6\rho\tilde{U}) G_1(j,k;t) = \delta(t)\delta_{r_j,r_k} - K \sum_{r_0} G_1(r_j+r_0,r_k;t) + \\ + \rho U_0 G_2(j,k;t) \end{aligned} \quad (3.19)$$

$$\begin{aligned} (i \frac{\partial}{\partial t} - 6K - 6\rho\tilde{U} - \rho U_0) G_2(j,k;t) = 2\delta(t)\delta_{r_j,r_k} - \\ - 2K \sum_{r_0} G_1(r_j+r_0,r_k;t) + K \sum_{r_0} G_1(j,k;t) \langle \phi_0 | b_{r_j+r_0}^* b_{r_j} | \phi_0 \rangle \end{aligned} \quad (3.20)$$

Of course, these equations are good approximations only if $n^2 - n$ is very small.

Solving this coupled pair of differential equations for $G_1(j,k;t)$:

$$\begin{aligned} (i \frac{\partial}{\partial t} - 6K - 6\rho\tilde{U}) (i \frac{\partial}{\partial t} - 6K - 6\rho\tilde{U} - \rho U_0) G_1(j,k;t) = \\ = (i \frac{\partial}{\partial t} - 6K - 6\rho\tilde{U} - \rho U_0) [(\delta(t)\delta_{r_j,r_k} - K \sum_{r_0} G_1(r_j+r_0,r_k;t))] \\ + \rho U_0 2\delta(t)\delta_{r_j,r_k} - 2\rho U_0 K \sum_{r_0} G_1(r_j+r_0,r_k;t) + \\ + \rho U_0 K \sum_{r_0} \langle \phi_0 | b_{r_j+r_0}^* b_{r_j} | \phi_0 \rangle G_1(j,k;t) \end{aligned} \quad (3.21)$$

Now

$$\frac{1}{N} \sum_k e^{ikx} e^{-ikx^1} = \delta_{x, x^1}$$

$$\frac{1}{N} \sum_x e^{ikx} e^{-ik^1 x} = \delta_{k, k^1}$$

which in the limit of an infinitely large box and infinitesimal cell size becomes:

$$\frac{r_o^3}{(2\pi)^3} \int e^{ikx} e^{ikx^1} d^3k = r_o^3 \delta(\vec{x} - \vec{x}^1) \quad (3.22)$$

The lower and upper limits of integration are $k_i = -\frac{\pi}{r_o}$ and $k_i = \frac{\pi}{r_o}$ and

$$\left(\frac{1}{r_o}\right)^3 \int_{-\infty}^{\infty} e^{ikx} e^{-ikx} dx^3 = \left(\frac{2\pi}{r_o}\right)^3 \delta(\vec{k} - \vec{k}^1)$$

where $k_i = k_x, k_y, k_z$.

Therefore if one defines:

$$G(k, t) = \left(\frac{1}{r_o}\right)^3 \int_{-\infty}^{\infty} G(\vec{r}_j - \vec{r}_k, t) e^{-i\vec{k} \cdot (\vec{r}_j - \vec{r}_k)} d^3k(\vec{r}_j - \vec{r}_k) \quad (3.23)$$

It follows that:

$$G(\vec{r}_j - \vec{r}_k, t) = \left(\frac{r_o}{2\pi}\right)^3 \int G(k, t) e^{i\vec{k} \cdot (\vec{r}_j - \vec{r}_k)} d^3k \quad (3.24)$$

One may consider for a moment the solution of equation (3.20) in the limit as $\rho \rightarrow \infty$ as a simple instructive case. Taking the limit equation (3.20) may be written as:

$$\begin{aligned}
(i \frac{\partial}{\partial t} - 6K - 6\rho \tilde{U}) (i \frac{\partial}{\partial t} - 6K - 6\rho \tilde{U} - \rho U_0) G_1(j,k;t) = \\
= (i \frac{\partial}{\partial t} - 6K - 6\rho \tilde{U} + \rho U_0) \delta(t) \delta_{r_j, r_k}
\end{aligned} \quad (3.25)$$

Making use of equation (3.24) and the initial condition that

$E_n(N+1) - E_0(N) \geq E_0(N) - E_n(N-1)$, where $E_n(N)$ is the n^{th} energy eigenvalue of a system of N particles, one obtains as the solution of (3.25):

$$G_1(k, \omega) = - \frac{1}{\omega - 6K - 6\rho \tilde{U} - i\eta} + \frac{2}{\omega - 6K - 6\rho U - \rho \tilde{U}_0 - i\eta} \quad (3.26)$$

and

$$G_1(r_j - r_k, t) = \begin{cases} -i e^{i(6K + 6\rho \tilde{U})t} \delta_{r_j, r_k} & \text{for } t < 0 \\ -2ie^{i(6K + 6\rho \tilde{U} + \rho U_0)t} \delta_{r_j, r_k} & \text{for } t > 0 \end{cases} \quad (3.27)$$

Thus, one obtains from equation (3.3)

$$\langle \varphi_0 | b_{r_j}^* b_{r_j} | \varphi_0 \rangle = \lim_{t \rightarrow 0^-} i G_1(r_j, r_j; t) \quad (3.28)$$

$$= 1$$

Also

$$\langle \varphi_0 | b_{r_j} b_{r_j}^* | \varphi_0 \rangle = \lim_{t \rightarrow 0^+} i G_1(j, j; t) \quad (3.29)$$

$$= 2$$

Either equation (3.26), or equation (3.27) imply that the energy of a single particle in the system, in the limiting case $\rho \rightarrow \infty$, is the

kinetic energy of localization $6K$ plus the potential energy due to the attraction of the six particles next to it. On the other hand, the energy of a particle added to the system is equal to the kinetic energy of localization plus the potential energy due to attraction plus the repulsive potential energy due to the other particle in the same cell.

Equation (3.20) can be rewritten, using equation (3.24), as follows:

$$\begin{aligned}
 (\omega - 6K - 6\rho\tilde{U})(\omega - 6K - 6\rho\tilde{U} - \rho U_0) G_1(k, \omega) = \\
 = (\omega - 6K - 6\rho\tilde{U} - \rho U_0) [1 - KG_1(k, \omega) \sum_{r_0} e^{ik \cdot r_0}] + 2\rho U_0 \\
 - 2K\rho U_0 G_1(k, \omega) \sum_{r_0} e^{ik \cdot r_0} + \rho U_0 k G_1(k, \omega) \sum_{r_0} \langle \varphi_0 | b_{r_j+r_0}^* b_{r_j} | \varphi_0 \rangle \quad (3.30)
 \end{aligned}$$

Some algebraic simplification of this expression yields:

$$(\omega - \omega_+)(\omega - \omega_-) G_1(k, \omega) = \omega - 6K - 6\rho\tilde{U} + \rho U_0 \quad (3.31)$$

where

$$\begin{aligned}
 \omega_{\pm} = 6K + \frac{\rho U_0}{2} - \frac{k}{2} \sum_{r_0} e^{ik \cdot r_0} + 6\rho\tilde{U} \pm \\
 \pm \sqrt{\frac{1}{2} \rho U_0 - \frac{k}{2} \sum_{r_0} e^{ik \cdot r_0}}^2 - \rho U_0 K \sum_{r_0} e^{ik \cdot r_0} + \rho U_0 K h \quad (3.32)
 \end{aligned}$$

where

$$h = \sum_{r_0} \langle \varphi_0 | b_{r_j+r_0}^* b_{r_j} | \varphi_0 \rangle \quad (3.33)$$

$$\text{Let } x = \frac{2K}{\rho U_0}$$

For values of x larger than x_0 ω_+ and ω_- are complex, where x_0 is given by:

$$(1 - 3x_0)^2 - 12x_0 + 12hx_0 = 0 \quad (3.34)$$

i.e. the value of x for which ω_{\pm} became complex.

h is given in Appendix B as

$$12(x) \quad (3.35)$$

Complex values of ω_+ and ω_- have no physical meaning. No such values would have been obtained if there were no approximations in the problem. The approximations used are good for a system with small fluctuations, i.e. a system in its solid state. If the system described here remained a solid for all values of ρ , then the results one would obtain would be very sensible. The fact that the results obtained for $x > x_0$, i.e. $\rho < \rho_0$, become nonsensical can be taken to imply that the system is not a solid at all densities. A good estimate of the transition density is ρ_0 . It is the best estimate afforded by this description anyway.

In the limit as $k \rightarrow 0$, the poles ω_{\pm} can be simplified, from equation (3.32)

$$\omega_{\pm} \rightarrow 6K + \frac{\rho U_0}{2} - 3K - \frac{K}{2} (kr_0)^2 - 6\rho \tilde{U}_{\pm} \quad (3.36)$$

$$\pm \sqrt{\left(\frac{1}{2} \rho U_0\right)^2 (1-3x)^2 - 12x + 12hx + \left(\frac{1}{2} \rho U_0\right)^2 \left[3(1-x) \frac{k^2}{m\rho U_0} + \frac{k^2}{2m\rho U_0}\right]}$$

For $x > x_0$ $\omega_{\pm} \rightarrow \text{Constant}_1 + \text{Constant}_2 k^2$. For $x = x_0$

$$(1 - 3x) - 12x + 12hx = 0 \quad \text{and} \quad \omega_{\pm} = \text{Constant}_3 + \text{Constant}_4 k \quad (3.37)$$

That is, as the density is lowered a point will be reached at which the energy spectrum becomes linear in momentum. It should be noticed that $\omega_+(k) = \epsilon_{N+1}(k) + \mu_{N+1}$ and $\omega_-(k) = \mu_N - \epsilon_N(k)$, where μ_N is the chemical potential and $\epsilon_N(k)$ is the excitation energy of a system of N particles. Therefore

$$\mu_N = 3K + \frac{\rho U_0}{2} + 6\rho \tilde{U} \quad \text{for } x = x_0 \quad (3.38)$$

and

$$\epsilon_N(k) \rightarrow \frac{1}{2} \sqrt{\rho U_0 \frac{3(1-x)}{m}} k \quad \text{as } k \rightarrow 0 \quad \text{for } x = x_0 \quad (3.39)$$

these results are very similar to those obtained by Gersch²⁵ and Knollman with no attractive interactions. The chemical potential obtained here differs from their results as should be expected due to the inclusion of the attractive interaction. The density of transition is, as obtained here, slightly different from their result.

On the other hand, the excitation spectrum for $x = x_0$ is exactly the same in both cases. Apparently the attractive interaction does not inhibit the energy spectrum typical of a superfluid. The pressure exerted by the system does depend on the attractive interaction in a way that will be shown in the next chapter. Thus a strong enough attractive interaction may inhibit the solid-fluid transition due to the fact that the pressure of the system may go to zero for a density with a larger value than that one obtained from equation (3.37). The following qualitative diagrams should clarify things somewhat.

Here ρ_0 stands for zero pressure and $|\mu_3| > |\mu_2| > |\mu_1|$ and m is the one particle mass. In the second diagram ρ_0 corresponds to a

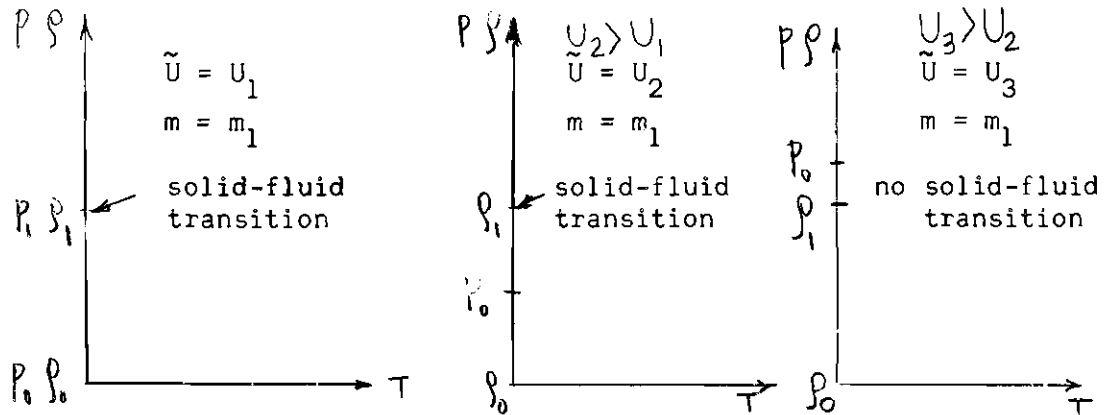


Figure 5. Dependence of the Solid-fluid Transition on the Attractive Interaction.

negative pressure. In the third diagram ρ_1 and ρ_0 correspond to a negative pressure.

On the other hand, if m changes then both the solid-fluid transition density and the zero pressure density change.

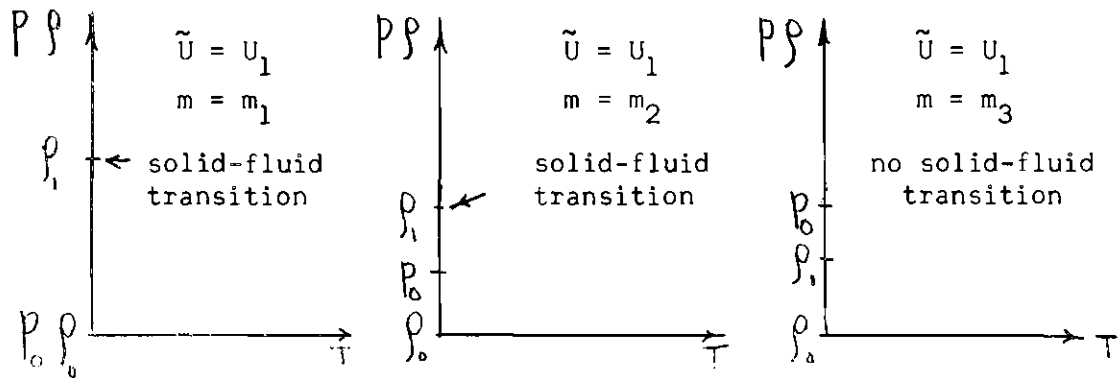


Figure 6. Dependence of the Solid fluid Transition on the Mass of the Particles.

where $m_3 > m_2 > m_1$. The dependence of $\rho(\rho_0)$ on the attractive interaction will be obtained in the next chapter.

Let a be the width of the two-particle potential interaction well, and let its depth be given by V . If these two particles are free in a large box their energy is about zero. If the two particles are bound together their energy is about $3 \frac{\pi^2 \hbar^2}{2ma^2} - V$. The particles will be free if $3 \frac{\pi^2 \hbar^2}{2ma^2} > V$. The same criterion is sometimes erroneously applied in the case of many particles in a box. If the density of the system in the ground state is very low the energy of a couple of bound particles is about $-V + 3 \frac{\pi^2 \hbar^2}{2ma^2}$, but if the particles are free their energy is about zero plus some small positive contribution from the repulsive interaction with other particles. Let this repulsive interaction be $f(\rho)$ with $\frac{df(\rho)}{d\rho} > 0$. Now consider a couple of particles in a high density system, i.e. the inter atomic distances are not very much larger than the atomic dimensions. Now the difference in energy between two systems, one with two particles bound and the other with the two particles free is about $-V + \frac{3\pi^2 \hbar^2}{2ma^2} - (-v + \tau + f(\rho))$ where $0 < \tau < \frac{3\pi^2 \hbar^2}{2ma^2}$, $-V < v < 0$ and $f(\rho) > 0$. $\tau > 0$ because the space available for the motion of this particle is not very large due to the presence of the other particles. $v \neq 0$ because the "free particle" feels the attraction of the other particles in the box to a significant degree due to their closeness. So if $f(\rho) - v + \tau < -V + \frac{3\pi^2 \hbar^2}{2ma^2}$, i.e. $f(\rho) + (V - v) < \frac{3\pi^2 \hbar^2}{2ma^2} - \tau$, the system will be in a fluid state. The larger the density the more important the role of the repulsive interactions become. For a large enough density $V - v$ becomes negligible as the results of this chapter suggest. This inequality shows the importance of $f(\rho)$ for large densities. For extremely high densities such as those dealt with in this work, a would have to be replaced by a smaller number.

CHAPTER IV

MORE REFINED TREATMENT OF BOSONS AT $T = 0$

The object of this chapter is to obtain a more accurate density of transition than the one previously obtained in equation (3.34). For this purpose some approximations will be refined. The relation pressure vs. density will be obtained to see if the pressure goes to zero before the system has a chance to undergo a phase transition, and thus obtain a criterion to know whether a system ought to be solid or fluid at $T = 0$, $p = 0$.

The following are exact dynamic equations (see Appendix A for evaluation of commutators):

$$\begin{aligned}
 (i \frac{\partial}{\partial t} - 6K) G_1(j, k; t) &= \delta_{r_j r_k} \delta(t) - K \sum_{r_0} G_1(r_j + r_0, r_k; t) - \\
 &- i \rho U_0 \langle \phi_0 | T b_{r_j}^*(t) b_{r_j}(t) b_{r_j}(t) b_{r_k}^*(0) | \phi_0 \rangle \\
 &- i \rho U \sum_{r_0} \langle \phi_0 | T b_{r_j + r_0}^*(t) b_{r_j + r_0}(t) b_{r_j}(t) b_{r_k}^*(0) | \phi_0 \rangle \quad (4.1)
 \end{aligned}$$

$$\begin{aligned}
 (i \frac{\partial}{\partial t} - 6k - \rho U_0) G_2(j, k; t) &= 2\delta_{r_j, r_k} \delta(t) + \\
 &+ 2Ki \sum_{r_0} \langle \phi_0 | T b_{r_j}^*(t) b_{r_j}(t) b_{r_j + r_0}(t) b_{r_k}^*(0) | \phi_0 \rangle \\
 &- iK \sum_{r_0} \langle \phi_0 | T b_{r_j + r_0}^*(t) b_{r_j}(t) b_{r_j}(t) b_{r_k}^*(0) | \phi_0 \rangle -
 \end{aligned}$$

$$\begin{aligned}
& - i \rho U_0 \langle \varphi_0 | T b_{r_j}^*(t) b_{r_j}^*(t) b_{r_j}(t) b_{r_j}(t) b_{r_j}(t) b_{r_k}^*(0) | \varphi_0 \rangle \\
& - i \rho \tilde{U} \sum_{r_0} \langle \varphi_0 | T b_{r_j}^*(t) b_{r_j}(t) b_{r_j}(t) b_{r_j+r_0}^*(t) b_{r_j+r_0}(t) b_{r_k}^*(0) | \varphi_0 \rangle \quad (4.2)
\end{aligned}$$

To improve the results obtained in the previous chapter the last term in equation (4.1) will not be approximated, as was done in equation (3.18), instead a new equation of motion will be obtained for it.

$$\begin{aligned}
\text{Let } \tilde{G}_2(j, k; t) &= -i \langle \varphi_0 | T b_{r_j+r_0}^*(t) b_{r_j+r_0}(t) b_{r_j}(t) b_{r_k}^*(0) | \varphi_0 \rangle \\
i \frac{\partial}{\partial t} \tilde{G}_2(r_j, r_k; t) &= \delta(t) (\delta_{r_j, r_k} + \langle \varphi_0 | b_{r_j+r_0} b_{r_j} | \varphi_0 \rangle \delta_{r_j+r_0, r_k}) - \\
& - i 6K \langle \varphi_0 | T b_{r_j+r_0}^*(t) b_{r_j+r_0}(t) b_{r_j}(t) b_{r_k}^*(0) | \varphi_0 \rangle \\
& - i \rho U_0 \langle \varphi_0 | T b_{r_j+r_0}^*(t) b_{r_j+r_0}(t) b_{r_j}^* b_{r_j} b_{r_j} b_{r_k}^*(0) | \varphi_0 \rangle \\
& - i \rho \tilde{U} \sum_{r'} \langle \varphi_0 | T b_{r_j+r_0}^*(t) b_{r_j+r_0}(t) b_{r_j}(t) b_{r_j+r'}^*(t) b_{r_j+r'}(t) b_{r_k}^*(0) | \varphi_0 \rangle \\
& + i K \sum_{r'} \langle \varphi_0 | T b_{r_j+r_0}^*(t) b_{r_j+r_0}(t) b_{r_j+r'} b_{r_k}^*(0) | \varphi_0 \rangle + \\
& + i K \sum_{r'} \langle \varphi_0 | T b_{r_j+r_0}^*(t) b_{r_j+r_0+r'}(t) b_{r_j} b_{r_k}^*(t) | \varphi_0 \rangle \\
& - i K \sum_{r'} \langle \varphi_0 | T b_{r_j+r_0+r'}^*(t) b_{r_j+r_0}(t) b_{r_j}(t) b_{r_k}^*(t) | \varphi_0 \rangle \quad (4.3)
\end{aligned}$$

Some approximations need to be made to solve this set of three coupled differential equations. The approximations must become exact in the limit as $\rho \rightarrow \infty$. The following approximations will be made:

$$\begin{aligned}
\sum_{\mathbf{r}'} \langle \varphi_0 | T b_{\mathbf{r}_j + \mathbf{r}'}^* (t) b_{\mathbf{r}_j} (t) b_{\mathbf{r}_j} (t) b_{\mathbf{r}_k}^* (0) | \varphi_0 \rangle &= \\
&= \sum_{\mathbf{r}'} \langle \varphi_0 | b_{\mathbf{r}_j + \mathbf{r}'}^* b_{\mathbf{r}_j} | \varphi_0 \rangle \langle \varphi_0 | T b_{\mathbf{r}_j} (t) b_{\mathbf{r}_k}^* (0) | \varphi_0 \rangle \quad (4.4)
\end{aligned}$$

$$\begin{aligned}
\sum_{\mathbf{r}'} \langle \varphi_0 | T b_{\mathbf{r}_j}^* (t) b_{\mathbf{r}_j} (t) b_{\mathbf{r}_j + \mathbf{r}'} (t) b_{\mathbf{r}_k}^* (0) | \varphi_0 \rangle &\simeq \\
&\simeq \sum_{\mathbf{r}'} \langle \varphi_0 | b_{\mathbf{r}_j}^* b_{\mathbf{r}_j} | \varphi_0 \rangle \langle \varphi_0 | T b_{\mathbf{r}_j + \mathbf{r}'} (t) b_{\mathbf{r}_k}^* (0) | \varphi_0 \rangle \quad (4.5)
\end{aligned}$$

$$\langle \varphi_0 | T b_{\mathbf{r}_j}^* (t) b_{\mathbf{r}_j}^* (t) b_{\mathbf{r}_j} (t) b_{\mathbf{r}_j} (t) b_{\mathbf{r}_j} b_{\mathbf{r}_k}^* (0) | \varphi_0 \rangle \simeq 0 \quad (4.6)$$

$$\begin{aligned}
\langle \varphi_0 | T b_{\mathbf{r}_j}^* (t) b_{\mathbf{r}_j} (t) b_{\mathbf{r}_j} (t) b_{\mathbf{r}_j + \mathbf{r}'}^* (t) b_{\mathbf{r}_j + \mathbf{r}'} (t) b_{\mathbf{r}_k}^* (0) | \varphi_0 \rangle &\simeq \\
&\simeq \sum_{\mathbf{r}'} \langle \varphi_0 | T b_{\mathbf{r}_j}^* (t) b_{\mathbf{r}_j} (t) b_{\mathbf{r}_j} (t) b_{\mathbf{r}_k}^* (0) | \varphi_0 \rangle \langle \varphi_0 | b_{\mathbf{r}_j + \mathbf{r}'}^* b_{\mathbf{r}_j + \mathbf{r}'} | \varphi_0 \rangle \quad (4.7)
\end{aligned}$$

$$\begin{aligned}
\sum_{\mathbf{r}'} \langle \varphi_0 | T b_{\mathbf{r}_j + \mathbf{r}'}^* (t) b_{\mathbf{r}_j + \mathbf{r}'} (t) b_{\mathbf{r}_j}^* (t) b_{\mathbf{r}_j} (t) b_{\mathbf{r}_j} (t) b_{\mathbf{r}_k}^* (0) | \varphi_0 \rangle &\simeq \\
&\simeq \sum_{\mathbf{r}'} \langle \varphi_0 | b_{\mathbf{r}_j + \mathbf{r}'}^* b_{\mathbf{r}_j + \mathbf{r}'} | \varphi_0 \rangle \langle \varphi_0 | T b_{\mathbf{r}_j}^* (t) b_{\mathbf{r}_j} (t) b_{\mathbf{r}_j} (t) b_{\mathbf{r}_k}^* (0) | \varphi_0 \rangle \quad (4.8)
\end{aligned}$$

$$\begin{aligned}
\sum_{\mathbf{r}'} \langle \varphi_0 | T b_{\mathbf{r}_j + \mathbf{r}_0}^* (t) b_{\mathbf{r}_j + \mathbf{r}_0} (t) b_{\mathbf{r}_j} (t) b_{\mathbf{r}_j + \mathbf{r}'}^* (t) b_{\mathbf{r}_j + \mathbf{r}'} (t) b_{\mathbf{r}_k}^* (0) | \varphi_0 \rangle &\simeq \\
&\simeq \sum_{\mathbf{r}'} \langle \varphi_0 | b_{\mathbf{r}_j + \mathbf{r}'}^* b_{\mathbf{r}_j + \mathbf{r}'} | \varphi_0 \rangle \langle \varphi_0 | T b_{\mathbf{r}_j + \mathbf{r}_0}^* (t) b_{\mathbf{r}_j + \mathbf{r}_0} (t) b_{\mathbf{r}_j} (t) b_{\mathbf{r}_k}^* (0) | \varphi_0 \rangle \quad (4.9)
\end{aligned}$$

$$\begin{aligned}
\sum_{\mathbf{r}'} \langle \varphi_0 | T b_{\mathbf{r}_j + \mathbf{r}_0}^* (t) b_{\mathbf{r}_j + \mathbf{r}_0} (t) b_{\mathbf{r}_j + \mathbf{r}'} (t) b_{\mathbf{r}_k}^* (0) | \varphi_0 \rangle &\simeq \\
&\simeq \sum_{\mathbf{r}' \neq \mathbf{r}_0} \langle \varphi_0 | b_{\mathbf{r}_j + \mathbf{r}_0}^* b_{\mathbf{r}_j + \mathbf{r}_0} | \varphi_0 \rangle \langle \varphi_0 | T b_{\mathbf{r}_j + \mathbf{r}'} b_{\mathbf{r}_k}^* (0) | \varphi_0 \rangle +
\end{aligned}$$

$$+ \langle \varphi_0 | T b_{r_j+r_0}^* (t) b_{r_j+r_0} (t) | \varphi_0 \rangle \langle \varphi_0 | b_{r_j+r'} (t) b_{r_k}^* (0) | \varphi_0 \rangle \quad (4.10)$$

$$\begin{aligned} \sum_{r'} \langle \varphi_0 | T b_{r_j+r_0}^* (t) b_{r_j+r_0+r'} (t) b_{r_j} (t) b_{r_k}^* (0) | \varphi_0 \rangle &\simeq \\ &\simeq \sum_{r'} \langle \varphi_0 | b_{r_j+r_0}^* b_{r_j+r_0+r'} | \varphi_0 \rangle \langle \varphi_0 | T b_{r_j} (t) b_{r_k}^* (0) | \varphi_0 \rangle \end{aligned} \quad (4.11)$$

$$\begin{aligned} \sum_{r'} \langle \varphi_0 | T b_{r_j+r_0+r'}^* (t) b_{r_j+r_0} (t) b_{r_j} (t) b_{r_k}^* (0) | \varphi_0 \rangle &\simeq \\ &\simeq \langle \varphi_0 | T b_{r_j} (t) b_{r_k}^* (0) | \varphi_0 \rangle (1 - \frac{1}{6} h) + \\ &+ \langle \varphi_0 | T b_{r_j+r'} (t) b_{r_k}^* (0) | \varphi_0 \rangle \end{aligned} \quad (4.12)$$

where

$$h = \sum_{r_0} \langle \varphi_0 | b_{r_j+r_0}^* b_{r_j} | \varphi_0 \rangle ; \quad \langle \varphi_0 | b_{r_j}^* b_{r_j} | \varphi_0 \rangle = 1$$

Approximations (4.4, 4.5 and 4.6) have already been used by Gersch²⁵ and Knallman. Notice should be taken of the fact that the approximations are as good for $t > t'$ as for $t < t'$, as it should be. To illustrate the spirit of the approximation equation (4.9) will be considered.

First for the case $t > 0$

$$\begin{aligned} \sum_{r'} \langle \varphi_0 | T b_{r_j+r_0}^* (t) b_{r_j+r_0} (t) b_{r_j} (t) b_{r_j+r'}^* (t) b_{r_j+r'} (t) b_{r_k}^* (0) | \varphi_0 \rangle &= \\ &= \sum_{r' \neq r_0} \langle \varphi_0 | T b_{r_j+r'}^* (t) b_{r_j+r'} (t) b_{r_j} (t) b_{r_j+r_0}^* (t) b_{r_j+r_0} (t) b_{r_k}^* (0) | \varphi_0 \rangle + \end{aligned}$$

$$+ \langle \phi_0 | b_{r_j+r_0}^*(t) b_{r_j+r_0}(t) b_{r_j}(t) b_{r_j+r_0}^*(t) b_{r_j+r_0}(t) b_{r_k}^*(0) | \phi_0 \rangle$$

since $[b_{r_j+r_0}^* b_{r_j+r_0} b_{r_j+r_0}^* b_{r_j+r_0} b_{r_j}]_- = 0$ if $r_j \neq r_0$.

It is clear then, that for $t > 0$ in the limiting case as $\rho \rightarrow \infty$ the approximation (4.9) becomes exact.

For the case $t < 0$

$$\begin{aligned} \langle \phi_0 | b_{r_k}^*(0) b_{r_j+r_0}(t) b_{r_j+r_0}(t) b_{r_j}(t) b_{r_j+r_0}^*(t) b_{r_j+r_0}(t) | \phi_0 \rangle = \\ = \sum_{r'} \langle \phi_0 | b_{r_j+r'}^* b_{r_j+r'} | \phi_0 \rangle \langle \phi_0 | b_{r_k}^*(0) b_{r_j+r_0}(t) b_{r_j+r_0}(t) b_{r_j}(t) | \phi_0 \rangle \end{aligned}$$

This approximation clearly becomes exact as $\rho \rightarrow \infty$. Every other approximation (from equation 4.4 to 4.12) satisfy the same requirement.

The new dynamical equations for $G_1(j,k;t)$, $G_2(j,k;t)$ and $G_2(j,k,t)$ making use of equations (4.4) to 4.12), are:

$$\begin{aligned} (i \frac{\partial}{\partial t} - 6K) G_1(j,k;t) = \delta_{r_j, r_k} \delta(t) - K \sum_{r'} G_1(r_j+r', r_k; t) \\ + \rho U_0 G_2(j,k;t) + \rho \tilde{U} \sum_{r_0} G_2(j,k;t) \end{aligned} \quad (4.13)$$

$$\begin{aligned} (i \frac{\partial}{\partial t} - 6K - 6\rho \tilde{U} - \rho U_0) G_2(j,k;t) = 2\delta_{r_j, r_k} \delta(t) - \\ - 2K \sum_{r'} G_1(r_j+r', k; t) - nKG_1(j,k;t) \end{aligned} \quad (4.14)$$

$$\begin{aligned}
(i \frac{\partial}{\partial t} - 6K - 6\rho U) \sum_{r_0} \tilde{G}_2(r, k; t) = & \delta(t) [6\delta_{r_j r_k} + \\
& + \sum_{r_0} \delta_{r_j+r_0, r_k} \varphi_0 [b_{r_j+r_0}^* b_{r_j} \varphi_0] + 6\rho U_0 G_2(j, k; t) - \\
& - \frac{\hbar}{6} K \sum_{r^0} \sum_{r^1} G_1(r_j+r_0+r^1, r_k; t) + 5\hbar K G_1(j, k; t) + \\
& + K \sum_{r_0} G_1(r_j+r_0, k; t) - 6K \sum_{r^1 \neq r_0} G_1(r_j+r^1, r_k; t) - \\
& - K \sum_{r^1} G_2(r_j+r^1, r_k; t)
\end{aligned} \quad (4.15)$$

Comparing equations (4.13) and (4.15) one notices that for $x = 0$

$\sum_{r_0} G_1(j, k; t) = 6G_1(j, k; t)$, which is the approximation used in the preface to chapter for $\tilde{G}_2(j, k; t)$.

Solving equations (4.13), (4.14) and (4.15) for $G_1(j, k, \tau)$ we obtain

$$\begin{aligned}
(i \frac{\partial}{\partial t} - 6K)(i \frac{\partial}{\partial t} - 6K - 6\rho \tilde{U})(i \frac{\partial}{\partial t} - 6K - 6\rho \tilde{U} - \rho U_0) G_1(j, k; t) = \\
= \delta_{r_j r_k} (i \frac{\partial}{\partial t} - 6K - 6\rho \tilde{U})(i \frac{\partial}{\partial t} - 6K - 6\rho \tilde{U} - \rho U_0) \delta(t) - \\
- (i \frac{\partial}{\partial t} - 6\rho \tilde{U})(i \frac{\partial}{\partial t} - 6K - 6\rho \tilde{U} - \rho U_0) K \sum_{r^1} G_1(r_j+r^1, r_k; t) + \\
+ \rho U_0 (i \frac{\partial}{\partial t} - 6K) (2\delta_{r_j r_k} - 2K \sum_{r^1} G_1(r_j+r^1, r_k; t) + K n G_1(r_j, r_k, t)) \\
+ \rho \tilde{U} (i \frac{\partial}{\partial t} - 6K - 6\rho \tilde{U} - \rho U_0) (6\delta_{r_j r_k} \delta(t) + \frac{\hbar}{6} \sum_{r^1} \delta_{r_j+r^1, r_k} \delta(t))
\end{aligned}$$

$$\begin{aligned}
& - K \frac{\hbar}{6} \sum_{r'} \sum_{r_0} G_1(r_j + r_0 + r', r_k; t) + 5\hbar K G_1(r_j, r_k; t) + \\
& + K \sum_{r_0} G_1(r_j + r_0, r_k; t) - 6K \sum_{r' \neq r_0} G_1(r_j + r', r_k; t) - \\
& - K \tilde{U} \sum_{r'} (2\delta_{r_j + r', r_k} \delta(t) - 2K \sum_{r''} G_1(r_j + r' + r'', r_k; t) + \\
& + Kg(r') G_1(r_j + r', r_k; t))
\end{aligned} \quad (4.16)$$

where

$$g(r') = \sum_{r''} \langle \varphi_0 | b_{r_j + r' + r''}^* b_{r_j} | \varphi_0 \rangle \quad (4.17)$$

Substituting for $G_1(j, k; t) = \frac{r_0^3}{(2\pi)^4} \int G_1(k, \omega) e^{i\vec{k} \cdot (\vec{r}_j - \vec{r}_k)} e^{-i\omega t} d^3k d\omega$

one obtains for $G(k = 0, \omega)$:

$$\begin{aligned}
& \varepsilon(\varepsilon - 6\rho\tilde{U})(\varepsilon - 6\rho\tilde{U} - \rho U_0) + (\varepsilon - 6\rho\tilde{U})(\varepsilon - \rho U_0 - 6\rho\tilde{U})6K + \\
& + 12K\rho U_0\varepsilon - \hbar K\rho U_0\varepsilon + \rho\tilde{U}(\varepsilon - 6\rho\tilde{U} - \rho U_0)(6\hbar K - 5\hbar K - 6K + 30K) + \\
& + K\rho\tilde{U}[-2K(36) = K \sum_{r'} g(r')] \quad G_1(k, \omega) = \\
& = (\omega - 6K - 6\rho\tilde{U})(\omega - 6K - 6\rho\tilde{U} - \rho U_0) + 2\omega\rho U_0 - 12K\rho U_0 + \\
& + \rho\tilde{U}(\omega - 6K - 6\rho\tilde{U} - \rho U_0)(6 + \frac{\hbar}{6} \sum_{r'} e^{i\vec{k} \cdot \vec{r}'} - 2K\tilde{U} \sum_{r'} e^{i\vec{k} \cdot \vec{r}'} \quad (4.18)
\end{aligned}$$

where

$$\varepsilon = \omega - 6K; \quad \text{let } y = \frac{6\tilde{U}}{U_0}, \quad a = \frac{\varepsilon}{\rho U_0} - y.$$

The equation to be solved to obtain the poles of $G_1(k, \omega)$ is obtained from (4.18). If equation (4.18) is divided by $(\rho U_0)^3$ one obtains after some simplification:

$$\begin{aligned} a^3 + (y + 3x - 1)a^2 + (3x - y + 2xy - \frac{h}{2}x + \frac{1}{2}hxy)a + \\ + 4xy - \frac{7}{12}hxy + x^2y \left[3 - \sum_{r'} \frac{g(r')}{24} \right] = 0 \end{aligned} \quad (4.19)$$

It is desired to know the values of x and y , i.e. $\frac{K}{\rho U_0}$ and $\frac{\tilde{U}}{U_0}$, for which the solutions of (4.19) become complex, i.e. the values of x and y for which there is an instability. The value of h is found in Appendix C to be $12x(1 + y)$. As for the value of $g(r')$, it is sufficient to know that $\sum_{r'} g(r') \sim 1$.

It is not easy to solve equation (4.19) for a . There is an equation rather similar to (4.19) for which the exact solution can be obtained easily. That equation is

$$a^3 + (y + 3x - 1)a^2 + (3x - y + 3xy - \frac{h}{2}x)a + 3xy - \frac{h}{2}xy = 0 \quad (4.20)$$

The solutions of equation (4.20) are

$$\begin{aligned} a_1 &= -y \\ a_{\pm} &= \frac{1}{2} \left[1 - 3x \pm \sqrt{(1 - 3x)^2 - 12x + 2xh} \right] \end{aligned}$$

That is, the solutions to equation (4.20) become complex for $x \gtrsim 0.06$

It will be shown later that the values of interest for y range

from 0 to -.1. With this in mind, and the solution of equation (4.20), with the condition that $x \lesssim .06$, one sees that equations (4.20) and (4.19) are almost identical.

The solutions of equation (4.19) should become complex at approximately the same value of x , $x \simeq .06$. To make sure that this is so a plot will be made of the function

$$f(\alpha) = \alpha^3 + (y + 3x - 1)\alpha^2 + (3x - y + 2xy - \frac{h}{2}x + \frac{1}{2}hxy)\alpha + 4xy - \frac{7}{12}hxy + x^2y \left[\left(3 - \sum_{r'} \frac{q(r')}{24} \right) \right] \quad (4.21)$$

for some values of x and y . For some values of x and y $f(\alpha)$ will have three real zeros, i.e. it will intercept the α axis; for other values of x and y $f(\alpha)$ will not intercept the α axis, i.e. the solutions of $f(\alpha) = 0$ are complex. Figures 7 and 8 indicate that for $|y| = \left| \frac{U}{U_0} \right| < .1$ the solutions of $f(\alpha) = 0$ become complex for $x \gtrsim .06$, just as expected.

The limitation that $|y| < .1$ does not restrict these results to systems with weak molecular attractions, as it might appear at first glance. If one wants to obtain the most stable configuration of a system of particles at high densities one compares the energies associated with each configuration and favors the configuration with the lowest energy. Two possible configurations are: one particle in each cell

$$E = (6K + 3\rho \tilde{U}) N$$

or two particles per cell packed compactly into one half the previous volume. The energy for this configuration would be

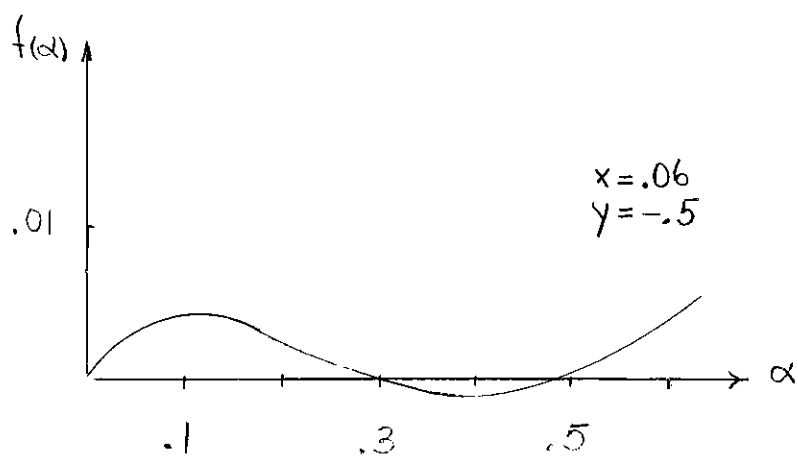
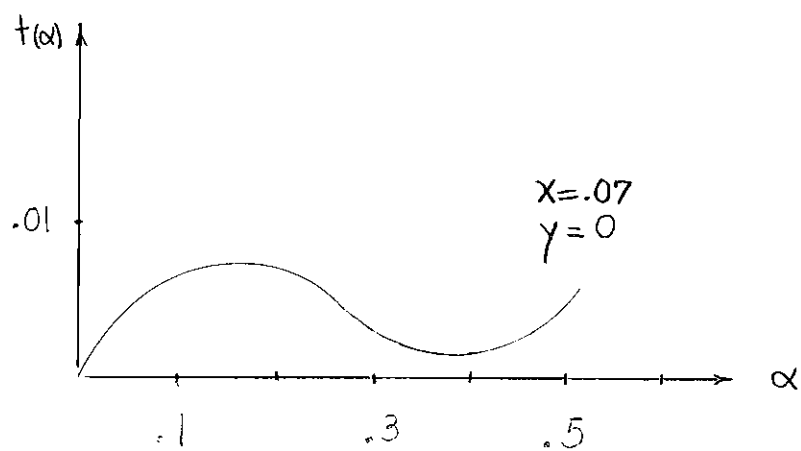
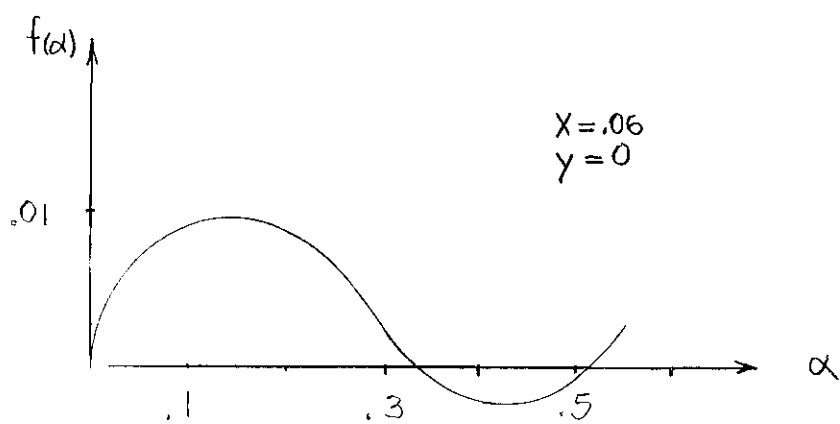


Figure 7. Values of x and y for Which ω_{\pm} Become Complex.

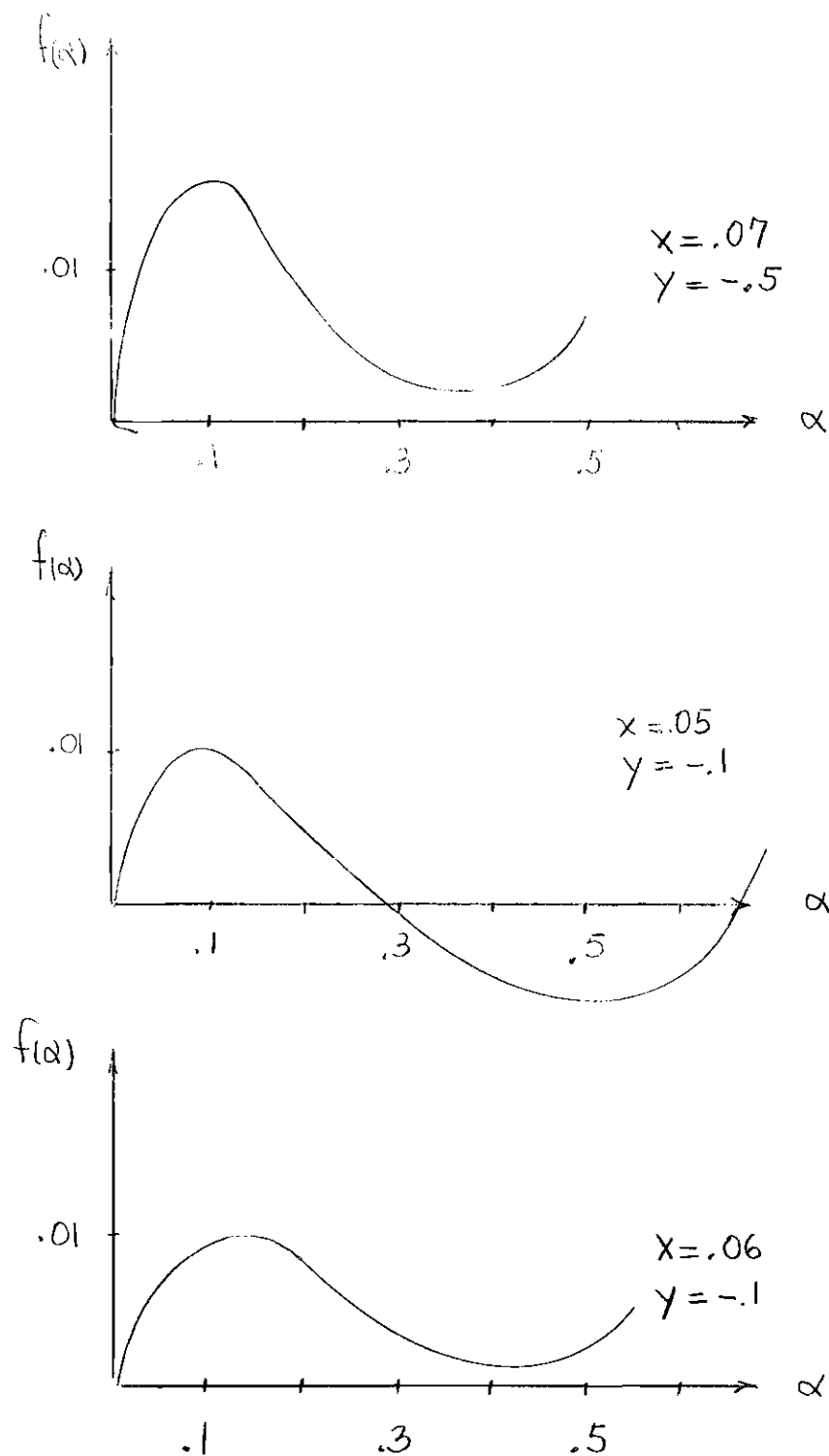


Figure 8. Values of x and y for Which ω_{\pm} Become Complex.

$$E = (6K + \frac{1}{2} \rho U_0 + 6 \rho \tilde{U})N. \quad (4.22)$$

Now $\rho \tilde{U} < 0$, so for the first configuration to be more stable than the second one it is necessary that:

$$\frac{1}{2} \rho U_0 + 6 \rho \tilde{U} > 3 \rho \tilde{U}$$

or

$$\frac{|\tilde{U}|}{U_0} < \frac{1}{6} \quad (4.23)$$

Then, the results valid for $|y| \lesssim .1$ should be applicable to all substances.

Now it is necessary to obtain the pressure as a function of density to find out if the pressure vanishes while the system is still in its solid state or not, i.e. if there is a solid-fluid transition or not.

The pressure will be obtained in the form of an expansion in powers of x . For this purpose the energy of the system will be first obtained, then making use of the relation

$$p = -\left(\frac{\partial E}{\partial V}\right)_s \quad (4.24)$$

the pressure will be obtained. It should be noticed that one is dealing with ground state energies in this problem, therefore the entropy, s , is zero for all values of the volume.

$$\begin{aligned} E = \langle \Phi_0 | H | \Phi_0 \rangle &= N 6 K i G_1(j, j; t=0^-) - i N K \sum_{r'} G_1(j, r_j + r'; t=0^-) + \\ &+ \frac{1}{2} N \rho U_0 i G_2(j, j; t=0^-) + \frac{1}{2} N \rho \tilde{U} \sum_{r'} G_2(j, j; t=0^-) \end{aligned} \quad (4.25)$$

From equation (4.1) one can write

$$\rho U_0 G_2(j, k; t) + \rho \tilde{U} \sum_{r_0} G_2(j, k, t) = (i \frac{\partial}{\partial t} - 6K) G_1(j, k; t) + \\ + K \sum_{r_0} G_1(r_j + r_0, r_k; t) .$$

The term $\delta_{r_j r_k} \delta(t)$ is omitted because in the evaluation of the energy one is concerned with the limits of the Green functions as $t \rightarrow 0$ not in the point $t = 0$.

Taking the Fourier transform of the previous expression one obtains

$$\rho U_0 G_2(j, k; \omega) + \rho \tilde{U} \sum_{r_0} G_2(j, k; \omega) = (\omega - 6K) G_1(j, k; \omega) + \\ + K \sum_{r_0} G_1(r_j + r_0, r_k; \omega)$$

Substituting this expression into equation (4.25) one obtains

$$E = \langle \Phi_0 | H | \Phi_0 \rangle = N \left(-\frac{1}{2} \frac{\partial}{\partial t} + i 3K \right) G_1(j, j; t=0^-) - \\ - N \frac{i}{2} K \sum_{r'} G_1(r_j, r_j + r'; t=0^-) \quad (4.26)$$

If equation (C.1), in the Appendix, is substituted into (4.26) the following expression for the energy is obtained:

$$E = iN \left[\frac{1}{2\pi} \int \frac{\omega}{2} G_1^{(0)}(j, j, \omega) + K G_1^{(1)}(j, j; \omega) + \omega e^{-i\omega 0} d\omega + \right. \\ \left. + (-i) 3K + i \frac{K}{2} 12(x + xy) \right] \quad (4.27)$$

where only the first two terms in the expansion of G_1 were used.

The previous equation is correct to first power in x . It is clear by looking at equation (C.6) that:

$$\int G_1^{(1)}(j, j; \omega) e^{-i\omega\tau} d\omega = 0 \quad (4.28)$$

The only task to be performed now is the evaluation of the integral

$$\int \frac{\omega}{2} G_1^{(0)}(j, j; \omega) e^{-i\omega\tau} d\omega$$

$G_1^{(0)}$ is obtained in Appendix C (equation (C.3))

$$G_1^{(0)}(j, k; \omega) = \left(-\frac{1}{\omega - 6K - 6\rho\tilde{U} - i\eta} + \frac{2}{\omega - 6K - 6\rho\tilde{U} - \rho U_0 + i\eta} \right) \delta_{j,k} \quad (4.29)$$

Therefore:

$$\int \frac{\omega}{2} G_1^{(0)}(j, j; \omega) e^{-i\omega\tau} d\omega = -2\pi i \frac{(6K + 6\rho\tilde{U})}{2} \quad (4.30)$$

It follows then that:

$$E = N (6K + 3\rho\tilde{U} - \frac{K}{2} 12x(1+y)) \quad (4.31)$$

Now, the kinetic energy, T , is:

$$T = \sum_{r_j} \langle \Phi_0 | b_{r_j}^* b_{r_j} | \Phi_0 \rangle 6K - K \sum_{r_j, r_0} \langle \Phi_0 | b_{r_j}^* b_{r_j+r_0} | \Phi_0 \rangle \quad (4.32)$$

as follows from equation (2.13).

But

$$\langle \Phi_0 | b_{r_j}^* b_{r_j} | \Phi_0 \rangle = 1 \quad \text{and} \quad \sum_{r_0} \langle \Phi_0 | b_{r_j}^* b_{r_j+r_0} | \Phi_0 \rangle = h = 12x(1+y)$$

Therefore

$$T = N[6K - K/2 x(1 + y)] \quad (4.33)$$

Now from (4.34) $p(p=0)$ may be found by solving:

$$V = E - T = (3\rho\tilde{U} + \frac{K}{2} x(1 + y))N \quad (4.34)$$

which may also be written in a more suggestive form as:

$$V = N[3\rho\tilde{U} + 3x^2 \rho U_0 + 3x^2 \rho\tilde{U}]$$

An expression for the pressure is now obtained.

$$p = - \frac{\partial E}{\partial V}$$

and

$$\frac{\partial E}{\partial V} = \frac{\partial E}{\partial p} \frac{\partial p}{\partial V}$$

but

$$\frac{\partial p}{\partial V} = - \frac{N}{V^2}$$

therefore

$$p = \frac{\partial E}{\partial p} \frac{1}{V} \quad (4.35)$$

So

$$p = \frac{1}{N} \frac{1}{V^2} \left[6 \frac{\partial K}{\partial p} + 3 \frac{\partial(\rho\tilde{U})}{\partial p} - \frac{\partial}{\partial p} \left(\frac{K}{2} x \frac{2K}{\rho U_0} \left(1 + \frac{\tilde{U}}{U_0} \right) \right) \right] \quad (4.36)$$

Clearly, for small x , the first two terms are dominant. Therefore

$$p \simeq \frac{1}{N} \rho^2 \left(\frac{\partial}{\partial \rho} E_{zp} + \frac{3\theta}{\partial \rho} (\rho \tilde{U}) \right) \quad (4.37)$$

where E_{zp} is the zero point energy $6K = 6 \frac{h^2 \rho^{2/3}}{2m}$

$$\frac{\partial}{\partial \rho} [6K + 3\rho \tilde{U}] = 0 \quad \text{with} \quad K = \frac{h^2 \rho^{2/3}}{2m}, \quad \tilde{U} < 0 \quad (4.38)$$

and compared with the solution of:

$$\frac{h^2 \rho^{2/3}}{m p U_0} = .06 \quad (4.39)$$

It is clear that $\rho(p=0)$ decreases as m decreases, while the value of ρ from equation (4.39) i.e. density of transition increases as m decreases. On the other hand, $\rho(p=0)$ decreases as $|\tilde{U}|$ decreases, but the solution of (4.39) is independent of \tilde{U} .

Equations (4.38) and (4.39) will now be applied to two cases. A system of He^4 molecules, and a system of Neon^{20} molecules. A simple cubic lattice is assumed for simplicity. The energy of localization will be computed assuming each particle is in an infinite square well. The volume of this three dimensional well will be (see Figure 9) $(2a)^3$. The energy of localization and potential energy as a function of the average intermolecular distance is shown in Figure 9 and Figure 10 for He^4 and Ne^{20} .

It is clearly seen that $\frac{K}{\rho U_0}$ is much smaller in the case of Neon than it is in the case of Helium, the values of K taken at the points where $p = 0$, i.e. $\frac{\partial}{\partial \rho} [6K + 3\rho \tilde{U}] = 0$; therefore the pressure went to zero too fast, in the case of Neon, to allow the kinetic energy to be large

enough compared with pU_0 for the system to become a fluid, if one assumes that He^4 goes into a fluid at a density slightly larger than $\rho(p=0)$, as is the case experimentally.

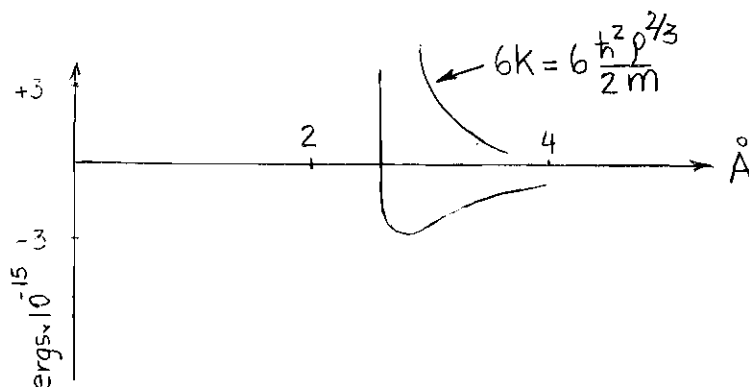


Figure 9. Zero Point Energy and Attractive Interaction vs. Molecular Distance for He^4 .

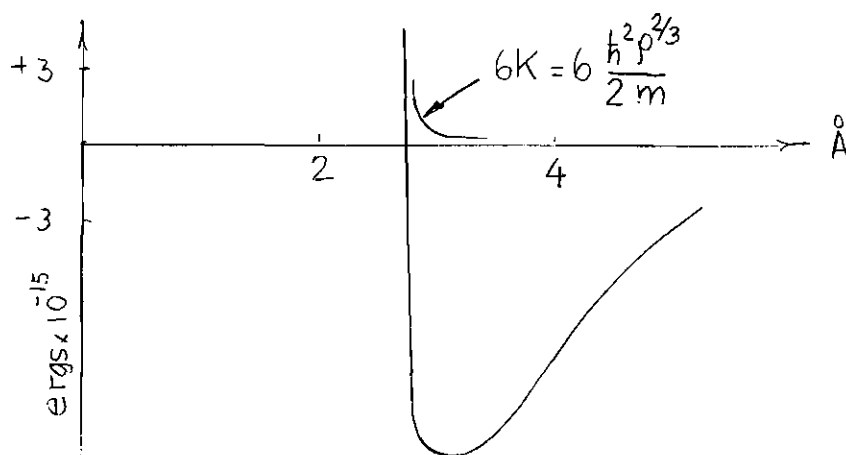


Figure 10. Zero point Energy and Attractive Interaction vs. Molecular Distance for Ne.

CHAPTER V

FERMIONS WITH REPULSIVE INTERACTIONS AT $T = 0$

A system of Fermi particles in the solid state at $T = 0$ with short range repulsive interactions will be considered in this chapter.

The interaction potentials of He^4 and He^3 atoms are not different. Their different behavior at $T = 0$ must be accounted for by the difference in statistics. A molecule of He^4 is a Bose particle whereas a molecule of He^3 is a Fermi particle.

Not much would be learned about the role of the statistics in this problem if both systems of Bosons and Fermions were to remain in the solid state at any pressure at $T = 0$, since the character of a solid is not very different from one case to the other. This is so because the effect of the exclusion principle for Fermions is of very little consequence in a solid since the dynamics of the system forbids any particle to go into a cell already occupied by one particle.

It will be shown, with the aid of Green functions in the cell model, that there is no solid-superfluid transition for Fermi particles. Some properties of the solid will also be studied.

The Hamiltonian, H , for a system of Fermions, is given by:

$$H = -\frac{\hbar^2}{2m} \sum_{\sigma} \int \Psi_{\sigma}^*(\mathbf{r}) \nabla^2 \Psi_{\sigma}(\mathbf{r}) d^3r + \frac{1}{2} \sum_{\sigma\sigma'} \iint \Psi_{\sigma}^*(\mathbf{r}) \Psi_{\sigma'}^*(\mathbf{r}') U(\mathbf{r}-\mathbf{r}') \Psi_{\sigma'}(\mathbf{r}') \Psi_{\sigma}(\mathbf{r}) d^3r d^3r' \quad (5.1)$$

where $\psi(r)$ annihilates one particle of spin σ at the point r , and obeys the usual anticommutation relations:

$$[\psi_\sigma(r), \psi_{\sigma'}^*(r')]_+ = \delta_{\sigma\sigma'} \delta(r-r') \quad (5.2)$$

and

$$[\psi_\sigma(r), \psi_{\sigma'}(r')]_+ = 0 \quad (5.3)$$

The operators $b_{\sigma r_j}$ and $b_{\sigma r_j}^*$ are defined by the relations

$$\psi_\sigma(r) = \rho^{1/2} \sum_{r_j} b_{\sigma r_j} \delta_{r_j, r} \quad (5.4)$$

where $\delta_{r_j, r} = \begin{cases} 1 & \text{if } r \text{ is within the } r_j^{\text{th}} \text{ cell} \\ 0 & \text{otherwise.} \end{cases}$

If one now chooses the volume of the cells to be $\frac{1}{\rho}$ one obtains from equations (5.2), (5.3) and (5.4) the following relations

$$\begin{aligned} [b_{\sigma r_j}, b_{\sigma' r_k}^*]_+ &= \delta_{\sigma\sigma'} \delta_{r_j, r_k} \\ [b_{\sigma r_j}, b_{\sigma' r_k}]_+ &= 0 \end{aligned} \quad (5.5)$$

Therefore $b_{\sigma r_j}$ destroys one particle with spin σ at the r_j^{th} cell.

Using equation (2.12) one can now write

$$\begin{aligned} \nabla^2 \rho^{1/2} \sum_{r_j} b_{\sigma r_j} \delta_{r_j, r} &= \rho^{1/2} \rho^{2/3} \left(-6 \sum_{r_j} b_{\sigma r_j} \delta_{r_j, r} + \right. \\ &\quad \left. + \sum_{r_j, r_0} b_{\sigma r_j} \delta_{r_j + r_0, r} \right) \end{aligned} \quad (5.6)$$

Substituting equations (5.4) and (5.6) into (5.1) one obtains:

$$H = -\frac{\hbar^2 p^2}{2m} \sum_{\sigma} \left(-6 \sum_{r_j} b_{\sigma r_j}^* b_{\sigma r_j} + \sum_{r_j, r_0} b_{\sigma r_j}^* b_{\sigma r_j + r_0} \right) + \\ + \frac{1}{2} p U_0 \sum_{\sigma, \sigma'} \sum_{r_j} b_{\sigma r_j}^* b_{\sigma' r_j}^* b_{\sigma' r_j} b_{\sigma r_j} \quad (5.7)$$

where $U_0 = p \int U(r-r') d\tau d\tau'$ and the range of interaction is assumed to be significantly smaller than the cell's dimensions.

The total spin operator, S , for the system commutes with the Hamiltonian. Therefore the ground state can be chosen to be an eigenfunction of S . It follows that

$$\langle \varphi_0 | T b_{\sigma r_j}(t) b_{\sigma' r_k}^*(0) | \varphi_0 \rangle = 0 \text{ if } \sigma \neq \sigma'.$$

With this fact in mind the one-particle Green function is defined as:

$$G_1(j, k; \sigma; t) = -i \langle \varphi_0 | T b_{\sigma r_j}(t) b_{\sigma r_k}^*(0) | \varphi_0 \rangle$$

where

$$T b_{\sigma r_j}(t) b_{\sigma r_k}^*(0) = \begin{cases} b_{\sigma r_j}(t) b_{\sigma r_k}^*(0) & \text{for } t > 0 \\ -b_{\sigma r_k}^*(t) b_{\sigma r_j}(t) & \text{for } t < 0 \end{cases} \quad (5.8)$$

As usual, the dynamical equation of the Green functions are sought.

$$i \frac{\partial}{\partial t} G_1(j, k; \sigma; t) = \left[\frac{\partial}{\partial t} \theta(t) \right] \langle \varphi_0 | b_{\sigma r_j}(t) b_{\sigma r_k}^*(0) | \varphi_0 \rangle - \quad (5.9)$$

$$- \left[\frac{\partial}{\partial t} \theta(t) \right] \langle \varphi_0 | b_{\sigma r_k}(0) b_{\sigma r_j}(t) | \varphi_0 \rangle + \langle \varphi_0 | T [b_{\sigma r_j}(t), H] b_{\sigma r_k}^*(0) | \varphi_0 \rangle$$

but

$$\frac{\partial}{\partial t} \theta(t) = \delta(t)$$

and

$$\frac{\partial}{\partial t} \theta(-t) = -\delta(t)$$

Therefore

$$i \frac{\partial}{\partial t} G_1(j, k; \sigma; t) = \delta(t) \delta_{r_j, r_k} + \langle \Phi_0 | T[b_{\sigma r_j}(t), H] b_{\sigma r_k}^*(0) | \Phi_0 \rangle \quad (5.10)$$

and making use of equation (D.5) one can finally write:

$$\begin{aligned} i \frac{\partial}{\partial t} G_1(j, k; \sigma; t) &= \delta(t) \delta_{r_j, r_k} + 6KG_1(j, k; \sigma; t) - \\ &- K \sum_{r'} G_1(r_j + r', r_k; \sigma; t) - \\ &- i\rho U_0 \langle \Phi_0 | T b_{\sigma', r_j}^*(t) b_{\sigma', r_j}(t) b_{\sigma r_j}(t) b_{\sigma r_k}^*(0) | \Phi_0 \rangle \end{aligned} \quad (5.11)$$

Let

$$G_2(j, \sigma'; k, \sigma; t) = -i \langle \Phi_0 | T b_{\sigma', r_j}^*(t) b_{\sigma', r_j}(t) b_{\sigma r_j}(t) b_{\sigma r_k}^*(0) | \Phi_0 \rangle \quad (5.12)$$

It should be noticed that σ' must be different from σ otherwise

$G_2(j, \sigma'; k, \sigma; t)$ equals zero. Every term in the equations for

$G_2(j, \sigma'; k, \sigma; t)$ is taken for $\sigma \neq \sigma'$. It is necessary to have a dynamical equation of $G_2(j, \sigma'; j, \sigma; t)$ in order to solve equation (5.11).

$$\begin{aligned}
i \frac{\partial}{\partial t} G_2(j, \sigma'; k, \sigma; t) = & \delta(t) \langle \Phi_0 | b_{\sigma', r_j}^*(t) b_{\sigma', r_j}(t) b_{\sigma r_j}(t) b_{\sigma r_k}^*(0) | \Phi_0 \rangle + \\
& + \delta(t) \langle \Phi_0 | b_{\sigma r_k}^*(0) b_{\sigma', r_j}^*(t) b_{\sigma', r_j}(t) b_{\sigma r_j}(t) | \Phi_0 \rangle \\
& + \langle \Phi_0 | T [b_{\sigma', r_j}^*(t) b_{\sigma', r_j}(t) b_{\sigma r_j}(t), H]_- b_{\sigma r_k}(0) | \Phi_0 \rangle \quad (5.13)
\end{aligned}$$

Now

$$\begin{aligned}
b_{\sigma', r_j}^*(0) b_{\sigma', r_j}(0) b_{\sigma r_j}(0) b_{\sigma r_k}^*(0) + b_{\sigma r_k}^*(0) b_{\sigma', r_j}^*(0) b_{\sigma', r_j}(0) b_{\sigma r_j}(0) = \\
= b_{\sigma', r_j}^*(0) b_{\sigma', r_j}(0) \delta_{r_j r_k} - b_{\sigma r_k}^*(0) b_{\sigma r_j}(0) + \\
+ b_{\sigma r_k}^*(0) b_{\sigma', r_j}^*(0) b_{\sigma', r_j}(0) b_{\sigma r_j}(0) = n_{\sigma'} \delta_{r_j, r_k}
\end{aligned}$$

With the aid of equation (D.9) one can now write equation (5.13) as:

$$\begin{aligned}
i \frac{\partial}{\partial t} G_2(j, \sigma'; k, \sigma; t) = & n_{\sigma'} \delta(t) \delta_{r_j, r_k} + 6KG_2(j, \sigma', k, \sigma; t) + \\
& + iK \sum_{r'} \langle \Phi_0 | T b_{\sigma', r_j}^*(t) b_{\sigma', r_j}(t) b_{\sigma r_{j+r'}}(t) b_{\sigma r_k}^*(0) | \Phi_0 \rangle + \\
& + iK \sum_{r'} \langle \Phi_0 | T b_{\sigma', r_j}^*(t) b_{\sigma', r_{j+r'}}(t) b_{\sigma r_j}(t) b_{\sigma r_k}^*(0) | \Phi_0 \rangle - \\
& - iK \sum_{r'} \langle \Phi_0 | T b_{\sigma', r_{j+r'}}^*(t) b_{\sigma', r_j}(t) b_{\sigma r_j}(t) b_{\sigma r_k}^*(0) | \Phi_0 \rangle + \\
& + p U_0 G_2(j, \sigma'; k, \sigma; t) \quad (5.14)
\end{aligned}$$

One respect in which this equation differs from the two particle Green function dynamical equation for Bosons is that no three particle Green function appears in this equation, $G_2(j, \sigma'; k, \sigma; t)$ is only coupled to other two particle Green functions.

This is so because in the three-particle Green function there would have to appear three destruction operators side by side, but from equation (5.5) it follows that $G_3 = 0$.

There is only one way to solve the coupled equations (5.11) and (5.14) without undertaking the terribly complicated task of finding the equations of motion of every two particle Green function appearing in equation (5.14), which in turn would contain new G_2 's, and then by making some approximations solve for G_1 . This is to approximate the two particle Green functions appearing in equation (5.14) by a product of G_1 's. This approximation should, of course, become asymptotically exact as $p \rightarrow \infty$. The only possible approximations are the following:

$$\begin{aligned} \sum_{r'} \langle \varphi_0 | T b_{\sigma', r_j}^*(t) b_{\sigma, r_j}(t) b_{\sigma, r_j+r'}(t) b_{\sigma, r_k}^*(0) | \varphi_0 \rangle &= \\ &= -h \langle \varphi_0 | T b_{\sigma, r_j}(t) b_{\sigma, r_k}^*(0) | \varphi_0 \rangle \end{aligned} \quad (5.15)$$

$$\begin{aligned} \sum_{r'} \langle \varphi_0 | T b_{\sigma', r_j+r'}^*(t) b_{\sigma, r_j}(t) b_{\sigma', r_j}(t) b_{\sigma, r_k}^*(0) | \varphi_0 \rangle &= \\ &= -\bar{h} \langle \varphi_0 | T b_{\sigma, r_j}(t) b_{\sigma, r_k}^*(0) | \varphi_0 \rangle \end{aligned} \quad (5.16)$$

$$\begin{aligned} \sum_{r'} \langle \varphi_0 | b_{\sigma', r_j}^*(t) b_{\sigma', r_j}(t) b_{\sigma, r_j+r'}(t) b_{\sigma, r_k}^*(0) | \varphi_0 \rangle &= \\ &= a \sum_{r'} \langle \varphi_0 | T b_{\sigma, r_j+r'}(t) b_{\sigma, r_k}^*(0) | \varphi_0 \rangle \end{aligned} \quad (5.17)$$

where $h = \sum_{r'} \langle \varphi_0 | b_{\sigma', r_j}^* b_{\sigma, r_j+r'} | \varphi_0 \rangle$ and $\bar{h} = \sum_{r'} \langle \varphi_0 | b_{\sigma', r_j+r'}^* b_{\sigma, r_j} | \varphi_0 \rangle$

where $a = 0$ for spins aligned, $a = 1$ for spins antialigned. It

may be worthwhile to examine the approximation of equation (5.17) in some detail. This approximation will be examined in the limit as $x \rightarrow 0$.

Suppose that $t < 0$ and the spins are aligned. Then the left side of equations (5.17) is zero and so is the right hand side. Now suppose that the spins are antialigned. Let $|\varphi\rangle$ be a normalized state function for a system with spin σ in the j^{th} cell and if the spin is σ' in the k^{th} cell then in all the adjacent cells the spin is σ' . Let $|\varphi\rangle$ be similar to $|\varphi_1\rangle$ in every respect except that if the spin in the 1^{th} cell in $|\varphi_1\rangle$ is σ then the spin in the 1^{th} cell in $|\varphi_2\rangle$ is σ' .

Due to the invariance to a translation through a cell spacing of the Hamiltonian one must have $|\varphi_0\rangle = \frac{1}{\sqrt{2}} |\varphi_1\rangle + \frac{1}{\sqrt{2}} |\varphi_2\rangle$ for antialigned spins.

Now if $r_k \neq r_j + r'$ then both the left and right side of equation (5.17) are zero. If $r_k = r_j + r'$ then the left side of equation (5.17) is either equal to $\langle \varphi_1 | \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} | \varphi_1 \rangle$ or $\langle \varphi_2 | \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} | \varphi_2 \rangle$ in either case equal to $\frac{1}{2}$. The right side of the equation is also equal to either $\langle \varphi_1 | \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} | \varphi_1 \rangle$ or $\langle \varphi_2 | \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} | \varphi_2 \rangle$ in either case equal to $\frac{1}{2}$.

Now $a = 1$ so both sides are equal again. Considering possible different approximations, such as:

$$\begin{aligned} \sum_{r'} \langle \varphi_0 | T b_{\sigma', r_j + r'}^* (t) b_{\sigma r_j} (t) b_{\sigma', r_j} (t) b_{\sigma r_k}^* (0) | \varphi_0 \rangle &= \\ &= \sum_{r'} \langle \varphi_0 | b_{\sigma', r_j + r'}^* b_{\sigma r_j} | \varphi_0 \rangle \langle \varphi_0 | T b_{\sigma', r_j} (t) b_{\sigma r_k}^* (0) | \varphi_0 \rangle \\ &= 0 \end{aligned}$$

because of different spin indices; one realizes that equations (5.15), (5.16) and (5.17) are the only suitable approximations.

The system under consideration is invariant to a translation through a cell spacing, therefore

$$\sum_{\mathbf{r}'} \langle \varphi_0 | b_{\sigma', \mathbf{r}_j}^* b_{\sigma', \mathbf{r}_j + \mathbf{r}'} | \varphi_0 \rangle = \langle \varphi_0 | b_{\sigma', \mathbf{r}_j + \mathbf{r}'}^* b_{\sigma', \mathbf{r}_j} | \varphi_0 \rangle \quad (5.18)$$

that is $\hbar = \bar{\hbar}$.

Then, it follows from equations (5.14), (5.15), (5.16) and (5.17) that:

$$\begin{aligned} (i \frac{\partial}{\partial t} - 6K - \rho U_0) G_2(j, \sigma'; k, \sigma; t) &= n_{\sigma'} \delta(t) \delta_{\mathbf{r}_j \mathbf{r}_k} - \\ &- aK \sum_{\mathbf{r}'} G_1(\mathbf{r}_j + \mathbf{r}', \sigma'; k, \sigma; t) \end{aligned} \quad (5.19)$$

Using

$$G_1(j, k; \sigma; t) = \frac{r_0^3}{(2\pi)^3} \frac{1}{2\pi} \int G_1(k, \omega; \sigma) e^{i\bar{k}(\bar{\mathbf{r}}_j - \bar{\mathbf{r}}_k)} e^{-i\omega t} d^3k d\omega$$

and

$$G_2(j, \sigma'; k, \sigma; t) = \frac{(r_0)^3}{(2\pi)^4} \int G_2(k, \omega; \sigma', \sigma) e^{i\bar{k}(\bar{\mathbf{r}}_j - \bar{\mathbf{r}}_k)} e^{-i\omega t} d^3k d\omega$$

one can write equations (5.11) and (5.19) as follows:

$$\begin{aligned} (\omega - 6K) G_1(k, \omega, \sigma) &= 1 - KG_1(k; \omega, \sigma) \sum_{\mathbf{r}'} e^{i\bar{k} \cdot \bar{\mathbf{r}}'} + \\ &+ \rho U_0 G_2(k, \omega; \sigma', \sigma) \end{aligned} \quad (5.20)$$

$$(\omega - 6K - \rho U_0) G_2(k, \omega; \sigma', \sigma) = n_{\sigma'} - aK G_1(k, \omega, \sigma) \sum_{\mathbf{r}'} e^{i\bar{k} \cdot \bar{\mathbf{r}}'} \quad (5.21)$$

Solving these two coupled equations for $G_1(k, \omega, \sigma)$ one gets:

$$G_1(k, \omega; \sigma) = \frac{\omega - 6K - \rho U_0(1 - n_{\sigma})}{\omega_+ - \omega_-} \left(\frac{1}{\omega - \omega_+} - \frac{1}{\omega - \omega_-} \right) \quad (5.22)$$

where

$$\omega_{\pm} = 6K + \frac{\rho U_0}{2} - \frac{K}{2} \sum_{r'} e^{i\vec{k} \cdot \vec{r}'} \pm \sqrt{\left(\frac{\rho U_0}{2} - \frac{K}{2} \sum_{r'} e^{i\vec{k} \cdot \vec{r}'} \right)^2 + \rho U_0 K \sum_{r'} e^{i\vec{k} \cdot \vec{r}'} (1-a) - i\eta} \quad (5.23)$$

Two simple cases will be studied briefly to illustrate some features of the result obtained.

Consider first the case of $n_{\sigma} = 0$, i.e. all the spins are lined up in the same direction.

$$\begin{aligned} \omega_+ &= 6K + \rho U_0 \\ \omega_- &= 6K - K \sum_{r'} e^{i\vec{k} \cdot \vec{r}'} \end{aligned} \quad \text{for } n_{\sigma} = 0 \quad (5.24)$$

Therefore

$$G_1(k, \omega; \sigma) = \frac{1}{\omega - 6K + K \sum_{r'} e^{i\vec{k} \cdot \vec{r}'} - i\eta} \quad (5.25)$$

There are no poles below the real axis, therefore $\langle \phi_0 | b_{\sigma k} b_{\sigma k}^* | \phi_0 \rangle = 0$, as it should be, because $|\phi_0\rangle$ is the state function for a system with one particle in every cell with spin up, so $b_{\sigma k} |\phi_0\rangle = 0$. On the other hand

$$n_{\sigma} = -\frac{i}{2\pi} \int G_1(k, \omega) e^{-i\omega 0^-} d\omega \quad (5.26)$$

With the expression for $G_1(k, \omega; \sigma)$ given in (5.25) one gets

$$n_{\sigma} = 1$$

consistent with the assumption that $n_{\sigma'} = 0$.

The second case to be considered is that of free fermions, i.e. $n_{\sigma} = 0$.

It is clear then, from equation (5.11), that:

$$G_1(k, \omega; \sigma) = \frac{\theta_1(k + k_f)}{\omega - \epsilon_K - k \sum_{r'} e^{i\vec{k} \cdot \vec{r}'} - i\eta} + \frac{\theta_2(k - k_f)}{\omega - \epsilon_K - k \sum_{r'} e^{i\vec{k} \cdot \vec{r}'} + i\eta} \quad (5.27)$$

$$\begin{aligned} \text{where } \theta_1(k + k_f) &= 1 & \text{for } 0 \leq k \leq k_f \\ &= 0 & \text{otherwise} \end{aligned}$$

$$\begin{aligned} \text{and } \theta_2(k - k_f) &= 1 & \text{for } k > k_f \\ &= 0 & \text{otherwise.} \end{aligned}$$

The value that one chooses for k_f determines how many particles will have spin σ and how many will have spin σ' . For example, for $k_f=0$ all the particles will have spin σ' . A value of k_f may be chosen, as will be shown in what follows so that $\frac{N}{2}$ particles have spin σ and $\frac{N}{2}$ have spin σ' .

$G_1(k, \omega; \sigma)$ as expressed in equation (5.27) is a solution of equation (5.11) regardless of the value of k_f . However equation (5.11) holds for any $|\phi\rangle$, i.e. the differential equation says nothing about the state in which the system is. The choice of the ground state is equivalent to the specification of some initial condition for the differential equation, i.e. the choice of k_f . If one chose $k_f = 0$, then

$$\begin{aligned}
& (\omega - 6K)(\omega - 6K - 6\rho\tilde{U})(\omega - 6K - 6\rho\tilde{U} - \rho U_0) G_1^{(1)}(j, k; \omega) + \\
& + (\omega - 6K - 6\rho\tilde{U})(\omega - 6K - 6\rho\tilde{U} - \rho U_0) \sum_{r'} G_1^{(0)}(r_j + r', r_k; \omega) + \\
& + 2\rho U_0(\omega - 6K) \sum_{r'} G_1^{(0)}(r_j + r'; r_k; \omega) - \\
& - \rho\tilde{U}(\omega - 6K - 6\rho\tilde{U} - \rho U_0) \left[\sum_{r'} G_1(r_j + r', r_k; \omega) + \right. \\
& \left. - 6 \sum_{r' \neq r_0} G_1^{(0)}(r_j + r', r_k; \omega) \right] = \rho\tilde{U}(\omega - 6K - 6\rho\tilde{U} - \rho U_0) \frac{h^{(1)}}{6} \sum_{r'} \delta_{r_j + r', r_k}
\end{aligned} \tag{C.5}$$

where $h^{(1)} = i \sum_{r'} G_1^{(1)}(r_j + r', r_j; 0^-)$

It follows from equation (5.5) that:

$$\begin{aligned}
G_1^{(1)}(j, k; \omega) = & -A^2(\omega) \sum_{r'} \delta_{r_j + r', r_k} + \frac{6\rho\tilde{U} A(\omega) \sum \delta_{r_j + r', r_k}}{(\omega - 6K - i\eta)(\omega - 6K - 6\rho\tilde{U} - i\eta)} + \\
& + \frac{\rho U A(\omega)}{(\omega - 6K - i\eta)(\omega - 6K - 6\rho\tilde{U} - i\eta)} \left[\sum_{r'} \delta_{r_j + r', r_k} - 6 \sum_{r'=1}^5 \delta_{r_j + r', k} \right] + \\
& \frac{\rho\tilde{U} \frac{h^{(1)}}{6} \sum_{r'} \delta_{r_j + r', r_k}}{(\omega - 6K - i\eta)(\omega - 6K - 6\rho\tilde{U} - i\eta)}
\end{aligned} \tag{C.6}$$

$$h^{(0)} = i \sum_{r'} G_1^{(0)}(r_j + r', r_j; 0) = \frac{i}{(2\pi)} \int G_1^{(0)}(r_j + r', r_j; \omega) e^{-i\omega 0^-} d\omega \tag{C.7}$$

It follows from equation (C.3) that:

$$h^{(0)} = 0 \tag{C.8}$$

$\langle \phi_0 | b_{\sigma_k}^* b_{\sigma_k} | \phi_0 \rangle = 0$, i.e. one would be specifying a system with all its particles with spin σ' . If one wants to talk about a system in the ground state one better choose k_f so that the energy is a minimum, i.e. $\frac{N}{2}$ particles with spin σ and $\frac{N}{2}$ particles with spin σ' . k_f is given by:

$$(N) \frac{(-i)(r_0)^3}{(2\pi)^4} \int \int_{k=0}^{|k|=k_f} G_1(k, \omega, \sigma) e^{-i\omega\tau} d^3k d\omega = \frac{N}{2}$$

$$\stackrel{N}{=} (r_0)^3 \frac{(-i)}{(2\pi)^4} \frac{1}{8} \int \int_{k=0}^{k^2=k_f^2} G_1(k, \omega, \sigma) e^{-i\omega\tau} 4\pi k^2 dk d\omega = \frac{N}{2}$$

whence

$$k_f = 2 (3\pi^2 \rho)^{1/3} \quad (5.28)$$

Now, the energy spectrum for a system of free Fermions is, from equation (5.27):

$$\begin{aligned} \omega &= 6K - K \sum_{\mathbf{r}_0} e^{i\mathbf{k} \cdot \mathbf{r}_0} \\ &= 6K - 6K + K \sum_{\mathbf{r}_0} (\mathbf{k} \cdot \mathbf{r}_0)^2 + \dots \\ &= \frac{\hbar^2}{2m} \sum_{i=1}^3 k_i^2 + \dots \end{aligned} \quad (5.29)$$

The correct energy spectrum is:

$$\omega = \sum_{i=1}^3 \frac{\hbar^2 k_i^2}{2m}$$

Equation (5.29) does not differ from the previous relation significantly for $k \ll r_0$, but these are particles with momentum up to k_f . It follows from equation (5.28) that there is a large range of momentum where the energy spectrum in the cell model differs strongly from the correct energy spectrum. The source of this discrepancy is the model itself. The set of orthogonal functions chosen as the set, kronecker delta functions, are not complete. This lack of completeness becomes noticeable when one wants to expand a function that varies significantly over the domain of a cell. One is dealing here with Fermions with momentum k larger than $\frac{1}{r_0}$, therefore one should expect to obtain a poor physical description in this model for these high momentum Fermions.

Now that these two special cases, $n_{\sigma} = 0$ and free Fermions, have been briefly examined the central problem in this chapter will be tackled, that is, whether the spins of the particles are aligned or anti-aligned.

If the spins in the presence of the short range repulsive interaction were aligned, then the energy of the system would be:

$$E = -i6K \sum_j G_1(j, j; \sigma; 0^-) + iK \sum_{r_j, r'} G_1(r_j + r', r_j; \sigma; 0^-)$$

From equation (5.25) one sees that

$$E = N 6 K \quad \text{for } n_{\sigma} = 0. \quad (5.30)$$

since $G_2(j, \sigma'; j, \sigma; t=0^-) = 0$ and

$$\sum_{\mathbf{r}'} -K \sum_{\mathbf{r}} \langle \phi_0 | b_{\mathbf{r}_j}^* b_{\mathbf{r}_j + \mathbf{r}'} | \phi_0 \rangle = +K i \frac{r_0^3}{(2\pi)^4} \int \frac{\sum_{\mathbf{r}_0} e^{i\mathbf{k} \cdot \mathbf{r}_0}}{\omega - 6K - \sum_{\mathbf{r}_0} e^{i\mathbf{k} \cdot \mathbf{r}_0} - i\eta} d\omega d^3k$$

where the limits of integration are $k_x, k_y, k_z = -\frac{\pi}{r_0}$ and $k_x, k_y, k_z = \frac{\pi}{r_0}$, and the integral in the previous expression equals zero, the energy is just $E = 6KN$

Now, if the spins are antialigned, then the energy is:

$$E = -i6K 2 \sum_{\mathbf{r}_j} G_1(j, j; \sigma; 0^-) + 2iK \sum_{\mathbf{r}_j, \mathbf{r}'} G_1(\mathbf{r}_j + \mathbf{r}', \mathbf{r}_j; \sigma; 0^-) + (i) \frac{1}{2} \rho U_0 G_2(j, \sigma'; j, \sigma; 0^-) \quad (5.31)$$

Now

$$G_2(j, \sigma'; j, \sigma; t=0^-) = \frac{1}{2\pi} \int G_2(j, \sigma'; j, \sigma; \omega) e^{-i\omega 0^-} d\omega$$

solving for $G_2(j, \sigma'; j, \sigma; \omega)$ in terms of $G_1(j, j; \omega; \sigma)$ in equation (5.20) and substituting into the previous expression one gets

$$\rho U_0 G_2(j, \sigma'; j, \sigma; t=0^-) = \frac{1}{2\pi} \int (\omega - 6K + K \sum_{\mathbf{r}_0} e^{i\mathbf{k} \cdot \mathbf{r}_0}) G_1(j, j; \omega; \sigma) e^{-i\omega 0^-} d\omega$$

Substituting the previous expression into equation (5.31) one obtains

$$E = i6K 2 \sum_{\mathbf{r}_j} G_1(j, j; \sigma; 0^-) + 2iK \sum_{\mathbf{r}_j, \mathbf{r}'} G_1(\mathbf{r}_j + \mathbf{r}', \mathbf{r}_j; \sigma; 0^-) + (-i) \frac{1}{2\pi} \int (\omega - 6K) G_1(j, j; \omega; \sigma) e^{-i\omega 0^-} d\omega +$$

$$\begin{aligned}
& + K \frac{(r_o)^3}{(2\pi)^4} \int G_1(k, \omega; r) \sum_{r'} i k \cdot r' e^{-i\omega\tau} d^3k d\omega \\
& = -i6K \sum_{r_j} G_1(j, j; \sigma, 0^-) + iK \frac{(r_o)^3}{(2\pi)^4} \int G_1(k, \omega; \sigma) \sum_{r'} e^{i\bar{k} \cdot \bar{r}'} e^{-i\omega\tau} d^3k d\omega
\end{aligned} \tag{5.22}$$

since $\int (\omega - 6k) G_1(j, j; \omega; \sigma) e^{-i\omega\tau} d\omega = 0$ with $a = 1$ as can be readily shown using equations (5.22) and (5.23). The integral

$$\frac{r_o^3}{(2\pi)^4} \int G_1(k, \omega; \sigma) \sum_{r'} e^{i\bar{k} \cdot \bar{r}'} e^{-i\omega\tau} d^3k d\omega$$

needs to be evaluated. With the aid of equations (5.22) and (5.23) the integral may be written as follows:

$$\begin{aligned}
& \frac{r_o^3}{(2\pi)^4} \int \frac{(\omega - 6K - \rho U_o \frac{1}{2})}{\rho U_o - K \sum_{r'} e^{i\bar{k} \cdot \bar{r}'}} \left(\frac{1}{\omega - 6K - \rho U_o + K \sum_{r'} e^{i\bar{k} \cdot \bar{r}'} + i\eta} - \right. \\
& \quad \left. - \frac{1}{\omega - 6K - i\eta} \right) \sum_{r'} e^{i\bar{k} \cdot \bar{r}'} d^3k d\omega \\
& = \frac{r_o (2\pi i)}{(2\pi)^4} \int \frac{\rho U_o \frac{1}{2}}{\rho U_o - K \sum_{r'} e^{i\bar{k} \cdot \bar{r}'}} \sum_{r'} e^{i\bar{k} \cdot \bar{r}'} d^3k
\end{aligned}$$

Expanding the denominator in series, for $\frac{K}{\rho U_o}$ small, and integrating one obtains

$$\frac{r_o^3}{(2\pi)^4} \int G_1(k, \omega, \sigma) \sum_{r'} e^{i\bar{k} \cdot \bar{r}'} e^{-i\omega\tau} d^3k d\omega = i \frac{3}{8} \times$$

therefore

$$E = N(6K - \frac{3}{8} x K)$$

Comparing this expression with the energy for the case of all spins aligned, equation (5.30), it is clear that the ground state corresponds to the spins antialigned.

It is of interest to note that:

$$G_2(j, j; \sigma, \sigma'; 0^-) = \frac{K}{\rho U_0} i \frac{3}{8} x$$

from equations (5.31), (5.32) and (5.33). But

$$G_2(j, \sigma'; j, \sigma; 0^-) = i \langle \phi_0 | n_{\sigma j} n_{\sigma' j} | \phi_0 \rangle$$

therefore

$$\langle \phi_0 | n_{\sigma' j} n_{\sigma j} | \phi_0 \rangle = \frac{3}{16} x^2$$

It is interesting to note, by inspecting equations (5.22) and (5.23), that there is no instability in the description of the system. The following argument shows that an instability in G_1 , obtained from a solution of two coupled differential equations, corresponds to a solid-superfluid transition, as opposed to a solid-normal fluid transition. The solution of a coupled pair of differential equations results in the solution of a second order differential equation, if each of the pair of equations is of first order. To obtain the poles of G_1 one has to solve a second order algebraic equation in ω . The instability occurs when ω_+ and ω_- become non real, i.e. $(\omega_+ - \omega_-) < 0$ for a certain value

of k and $\omega_+ - \omega_- \neq 0$ for all other values of k implies $n_k \rightarrow \infty$, but this only makes physical sense for $k = 0$. Now, if at the density for which $\omega_+(k=0) - \omega_-(k=0) = 0$ one makes an expansion about the point $k=0$, the first non zero term in the expansion is linear in k ; therefore for sufficiently small k $\epsilon(k)$ is linear in k ($\epsilon(k) = \frac{1}{2} \omega_+ - \omega_-$). It follows, then, that an instability in G_1 , where G_1 is the solution of a pair of coupled Green function equations, to be interpreted as a solid-normal fluid transition can never be obtained. In this light, it was to be expected that there would be no instability in G_1 for Fermions. If an instability is to be obtained in G_1 corresponding to a solid-normal fluid transition more than a pair of coupled differential equations for the Green functions must be solved or perhaps one needs a more refined model.

The main objective of this chapter is now fulfilled. It has been shown that a system of Fermions with the same interaction potential as a system of Bosons does not undergo a solid-superfluid transition, whereas the system of Bosons does.

One additional simple question will be considered. What is the strength of an externally applied magnetic field required to align the particle spins?

If the magnetic field B is aligned with the spin σ , then the Hamiltonian for the system is:

$$\begin{aligned}
 H = & 6K \sum_{r_j, \sigma} b_{\sigma r_j}^* b_{\sigma r_j} - K \sum_{r_j, \sigma, r'} b_{\sigma r_j}^* b_{\sigma r_j + r'} + \frac{U_0}{2} \sum_{r_j, \sigma, \sigma'} b_{\sigma' r_j}^* b_{\sigma' r_j} b_{\sigma r_j}^* b_{\sigma r_j} \\
 & - \mu B \sum_{r_j} b_{\sigma r_j}^* b_{\sigma r_j} + \mu B \sum_{r_j} b_{\sigma' r_j}^* b_{\sigma' r_j} \quad (5.35)
 \end{aligned}$$

let

$$H_B = -\mu B \sum_{r_j} b_{\sigma r_j}^* b_{\sigma r_j} + \mu B \sum_{r_j} b_{\sigma' r_j}^* b_{\sigma' r_j}$$

now

$$[b_{\sigma r_j}, H_B]_- = -\mu B b_{\sigma r_j}$$

and

$$[b_{\sigma' r_j} b_{\sigma' r_j} b_{\sigma r_j}, H_B]_- = -\mu B b_{\sigma' r_j} b_{\sigma' r_j} b_{\sigma r_j}$$

It follows that the new equations of motion for G_1 and G_2 are:

$$\begin{aligned} (i \frac{\partial}{\partial t} - 6K - \rho U_0 + \mu B) G_1(j, k; \sigma; t) &= \delta_{r_j, r_k} \delta(t) - \\ &- K \sum_{r'} G_1(r_j + r'; r_k; \sigma; t) + \rho U_0 G_2(j, \sigma'; k, \sigma; t) \end{aligned} \quad (5.36)$$

$$\begin{aligned} (i \frac{\partial}{\partial t} - 6K - \rho U_0 + \mu B) G_1(j, k; \sigma; t) &= n_{\sigma'} \delta_{r_j, r_k} \delta(t) - \\ &- a K \sum_{r'} G_1(r_j + r', r_k; \sigma; t) \end{aligned} \quad (5.37)$$

The solution is

$$G_1(k, \omega; \sigma) = \frac{\omega - 6K - \rho U_0 (n - n_{\sigma'}) + \mu B}{\omega_+ - \omega_-} \frac{1}{\omega - \omega_+} - \frac{1}{\omega - \omega_-} \quad (5.38)$$

$$\begin{aligned} \omega_{\pm} &= 6K + \frac{\rho U_0}{2} - K \sum_{r'} e^{i\vec{k} \cdot \vec{r}'} - \mu B \pm \\ &\pm \sqrt{\frac{\rho U_0}{2} - \frac{K}{2} \sum_{r'} e^{i\vec{k} \cdot \vec{r}'}^2 + \rho U_0 K \sum_{r'} e^{i\vec{k} \cdot \vec{r}'} (1-a)} \end{aligned} \quad (5.39)$$

All the poles are shifted by the same amount. Now if the spins are antialigned the energy of the system is:

$$E = N(6K - \frac{3}{8} \times K) \quad (5.40)$$

the energy of the system if the spins are all aligned is:

$$E = N(6K - \mu B) \quad (5.41)$$

The spins will all be aligned for

$$\mu B > \frac{3}{8} \times \frac{\hbar^2 p^{2/3}}{2m} \quad (5.42)$$

The weakest magnetic field necessary to align the spins is about 10^{10} gauss for $x \simeq .05$, $\frac{\hbar^2 p^{2/3}}{2m} \simeq 10$ degrees, and $\mu = \frac{e \hbar S}{2(\frac{m}{3})C}$.

Therefore, for all practical purposes the spins will never be aligned in solid He^3 at $T = 0$. Where C is the velocity of light.

CHAPTER VI

BOSONS WITH SHORT RANGE REPULSIVE INTERACTIONS AT $T \neq 0$ Introduction

A system of Bosons with very short range repulsive interaction at very low temperature will be treated in this chapter. The energy of the system, specific heat, fluctuations and density for the instability as a function of temperature will be calculated.

All the calculations will be done in the framework of the cell model. The approximations will be such that they will become exact asymptotically as $\rho \rightarrow \infty$ and $T \rightarrow 0$. The range of temperature for which the approximations are valid will be determined. The Green functions formalism as developed in Zubarev's³³ paper will be used. In this connection it should be noticed that $\mathcal{H} = H - \mu N$ will be used, as in Zubarev's paper, wherever H was used previously, because this simplifies the spectral theory to be used in the evaluation of thermodynamic quantities. The retarded and advanced Green functions, rather than the causal one, will be used.

The one-particle and two-particle Green functions will now be obtained. The retarded and advanced Green functions are defined as follows:

$$G_{1r}(j;k;t) = -i\theta(t) \langle\langle [b_{rj}(t), b_{rk}^*(0)]_- \rangle\rangle \quad (6.1)$$

$$G_{1a}(j;k;t) = i\theta(-t) \langle\langle [b_{rj}(t), b_{rk}^*(0)]_- \rangle\rangle \quad (6.2)$$

$$G_{2a}(j;k;t) = + i\theta(t) \langle\langle [b_{r_j}^*(t)b_{r_j}(t)b_{r_j}(t), b_{r_k}^*(0)]_- \rangle\rangle \quad (6.3)$$

$$G_{2r}(j;k;t) = i\theta(t) \langle\langle [b_{r_j}^*(t)b_{r_j}(t)b_{r_j}(t), b_{r_k}^*(0)]_- \rangle\rangle \quad (6.4)$$

where the double bracket, $\langle\langle \rangle\rangle$, signifies an average over the grand canonical ensemble, i.e.

$$\langle\langle A \rangle\rangle = \text{Trace} \langle \varphi_i | e^{-\frac{H}{\theta}} A | \varphi_i \rangle Z^{-1}; \quad Z^{-1} = \text{Trace} \langle \varphi_i | e^{-\frac{H}{\theta}} | \varphi_i \rangle$$

The equations of motion for G_{1a} and G_{1r}, G_{2a} and G_{2r} , are obviously the same, therefore the subscripts a and r will be omitted. The "grand-canonical Hamiltonian" is

$$H = (6K - \mu) \sum_{r_j} b_{r_j}^* b_{r_j} - K \sum_{r_j} b_{r_j}^* b_{r_j+r_o} + \frac{1}{2} \rho U_o \sum_{r_j} b_{r_j}^* b_{r_j}^* b_{r_j} b_{r_j}$$

The approximations used in this chapter will be different from those used in Chapter III. These approximations are

$$\begin{aligned} \langle\langle |Tb_{r_j}^*(t)b_{r_j}(t)b_{r_j+r_o}(t)b_{r_k}^*(0)| \rangle\rangle &= \\ &= \langle\langle |b_{r_j}^* b_{r_j}| \rangle\rangle \langle\langle |Tb_{r_j+r_o}(t)b_{r_k}^*(0)| \rangle\rangle \end{aligned} \quad (6.5)$$

$$\begin{aligned} \rho U_o \langle\langle |Tb_{r_j}^*(t)b_{r_j}^*(t)b_{r_j}(t)b_{r_j}(t)b_{r_j}(t)b_{r_k}^*(0)| \rangle\rangle + \\ + K 2 \langle\langle |Tb_{r_j}^*(t)b_{r_j+r_o}(t)b_{r_j}(t)b_{r_k}^*(0)| \rangle\rangle \simeq \\ \simeq K \gamma \langle\langle |Tb_{r_j}(t)b_{r_k}^*(0)| \rangle\rangle \end{aligned} \quad (6.6)$$

The reason why these approximations were made rather than those of Chapter III will become clear later. The constant γ will be evaluated later.

The validity of these approximations will be discussed later.

The equations of motion are:

$$[\omega - (6K - \mu)]G_1(j, k; \omega) = \delta_{r_j, r_k} - K \sum_{r'} G_1(r_j + r', r_k; \omega) + \rho U_0 G_2(r_j, r_k; \omega) \quad (6.7)$$

$$[\omega - (6K - \mu) - \rho U_0]G_2(j, k; \omega) = 2\delta_{r_j, r_k} - 2K \sum_{r'} G_1(r_j + r', r_k; \omega) + K\gamma G_1(j, k; \omega) \quad (6.8)$$

The solutions to these equations are:

$$G_1(k, \omega) = \frac{\omega - (6K - \mu) + \rho U_0}{\omega_+ - \omega_-} \left(\frac{1}{\omega - \omega_+ + \mu} - \frac{1}{\omega - \omega_- + \mu} \right) \quad (6.9)$$

$$G_2(k, \omega) = \frac{2[\omega - (6K - \mu)] + K\gamma}{\omega_+ - \omega_-} \left(\frac{1}{\omega - \omega_+ + \mu} - \frac{1}{\omega - \omega_- + \mu} \right) \quad (6.10)$$

$$\omega_{\pm} = 6K + \frac{1}{2} \rho U_0 \left(1 - x \sum_{r_0} \cos k \cdot r_0 \right) \pm \sqrt{\left(1 - x \sum_{r_0} \cos k \cdot r_0 \right)^2 - 4x \sum_{r_0} \cos k r_0 + 2x\gamma} \quad (6.11)$$

μ is the chemical potential for the system under consideration at temperature T and average number of particles N . An approximate equation will be used later which will in essence determine μ as a function of N and T , actually as a function of ρ and T with n_j chosen to be unity.

One must answer the following question now: To what extent are these approximations valid for $T \neq 0^\circ\text{K}$? The answer to this question will become more transparent if a bit of work is done for the simple case of $x = \frac{2K}{\rho U_0} \rightarrow 0$ computing $\langle\langle n_j \rangle\rangle$, keeping in mind that $\langle\langle n_j \rangle\rangle$ was already chosen to be unity in the Green's function equations. Thus $\mu(x=0, T)$ will be evaluated and light will be shed on the role of γ .

All quantities with a 0 superscript will be interpreted to be evaluated at $x = 0$.

From Zubarev's paper we have (eq. 3.28):

$$\langle\langle |a_k^+(t) a_k(t)| \rangle\rangle = - \frac{i}{2\pi} \int \frac{G_1(k; \omega - i\eta) - G_1(k; \omega + i\eta)}{e^{\frac{\omega}{\theta}} - 1} e^{-i\omega t} d\omega \quad (6.11)$$

and

$$g(k) = - \frac{i}{2\pi} \int \frac{G_2(k; \omega - i\eta) - G_2(k; \omega + i\eta)}{e^{\frac{\omega}{\theta}} - 1} d\omega \quad (6.11)$$

$$\text{where } n^2 - n \equiv \frac{r_0^3}{(2\pi)^3} \int g(k) d^3k \quad \text{defines } g(k). \quad (6.13)$$

and of course

$$\langle\langle |b_{r_k}^* b_{r_j}| \rangle\rangle = \left(\frac{r_0}{2\pi}\right)^3 \int \phi_0 |a_k^* a_k| \phi_0 e^{i\vec{k} \cdot (\vec{r}_j - \vec{r}_k)} d^3k \quad (6.14)$$

Now one requires that

$$\langle\langle |b_{r_j}^* b_{r_j}| \rangle\rangle = 1 \quad (6.15)$$

which implies

$$1 = \frac{(r_0)^3}{(2\pi)^3} \int \langle\langle |a_k^* a_k| \rangle\rangle d^3k \quad (6.16)$$

For $x = 0$

$$G_1^{(0)} = \frac{\omega - 6K + \mu + \rho U_0}{\rho U_0 \sqrt{1+2x\gamma}} \left(\frac{1}{\omega - 6K + \mu - \rho U_0 \left(\frac{1}{2} + \frac{1}{2}\sqrt{1+2x\gamma}\right)} - \frac{1}{\omega - 6K + \mu - \rho U_0 \left(\frac{1}{2} - \frac{1}{2}\sqrt{1+2x\gamma}\right)} \right) \quad (6.17)$$

It should be noticed that $x\gamma$ is not necessarily zero for $x = 0$ with the aid of equation (6.11) one gets:

$$\langle\langle |a_k^* a_k| \rangle\rangle = \left[- \frac{\frac{1}{6K - \mu + \rho U_0 \left(\frac{1}{2} - \frac{1}{2}\sqrt{1+2x\gamma}\right)}}{e^{\frac{\theta}{\theta}} - 1} + \frac{\frac{2}{6K - \mu + \rho U_0 \left(\frac{1}{2} + \frac{1}{2}\sqrt{1+2x\gamma}\right)}}{e^{\frac{\theta}{\theta}} - 1} \right] \frac{1}{\sqrt{1+2x\gamma}} \quad (6.18)$$

Equation (6.16) can now be written as:

$$1 = - \frac{\frac{1}{6K - \mu + \rho U_0 \left(\frac{1}{2} - \frac{1}{2}\sqrt{1+2x\gamma}\right)}}{e^{\frac{\theta}{\theta}} - 1} + \frac{\frac{2}{6K - \mu + \rho U_0 \left(\frac{1}{2} + \frac{1}{2}\sqrt{1+2x\gamma}\right)}}{e^{\frac{\theta}{\theta}} - 1} \frac{1}{\sqrt{1+2x\gamma}} \quad (6.19)$$

If $\langle\langle |a_k^* a_k| \rangle\rangle$ is to have finite values for all values of k , then equation (6.18) implies that $6K < \mu < 6K + \rho U_0$ for $\gamma x = 0$,

$$6K + \frac{1}{2} \rho U_0 (1 - \sqrt{1+2x\gamma}) < \mu < 6K + \frac{1}{2} \rho U_0 (1 + \sqrt{1+2x\gamma})$$

From equation (6.19) it follows that

$$x\gamma \simeq e^{\frac{6K - \mu + \frac{1}{2} \rho U_0 (1 - \sqrt{1+2x\gamma})}{\theta}} + 2e^{-\frac{6K - \mu + \rho U_0 (1 + \sqrt{1+2x\gamma})}{\theta}} \quad (6.20)$$

Of course, μ cannot in principle be completely determined from an equation with two unknowns γ and μ . It is important to notice that the equation $n_j = 1$ would not be satisfied for any value of μ had $x\gamma$ been chosen to be zero as was done at $T = 0^\circ K$ for $x = 0$. The reason for this is the following: at $x = 0$ the eigenstates of the Hamiltonian H are eigenstates of the operator n_j . The state with one particle per cell is the ground state. While the states with vacancies and double, triple, etc. occupancies are excited states. $h = \sum_{r'} \langle\langle b_{r_j}^+ b_{r_j+r'} | \rangle\rangle$ is proportional to the transition probability from a state of vacancy next to double occupancy to a state with one particle in each of those cells. $h \rightarrow 0$ as $x \rightarrow 0$ regardless of the value of T ; however $n^2 - n$ is different from zero for $x = 0$ if $\theta \neq 0$. This is why $\gamma \rightarrow 0$ as $x \rightarrow 0$ for $\theta = 0$ but $\gamma \not\rightarrow 0$ as $x \rightarrow 0$ for $\theta \neq 0$, because γ is a measure of h and $n^2 - n$.

For the case of $x = 0$ μ can be obtained easily by evaluating the grand partition function directly.

Let Z_g be the grand partition function

$$\begin{aligned} Z_g &= \sum_{\{n_j\}} e^{-\frac{1}{\theta} \left[6K \sum_j n_j - \mu \sum_j n_j + \frac{\rho U_0}{2} (n_j^2 - n_j) \right]} \\ &= \sum_{\{n_j\}} \prod_{j=1}^N e^{-\frac{1}{\theta} \left[(6K - \mu) n_j + \frac{\rho U_0}{2} (n_j^2 - n_j) \right]} \end{aligned} \quad (6.21)$$

where N is the number of cells for a particular sequence $\{n_j\}$ with

$$\sum n_j = N_0$$

The previous expression can be written as

$$\approx \sum_{n_j=0}^{\infty} \left[e^{-\frac{1}{\theta} \left[(6K-\mu)n_j + \frac{\rho U_0}{2} (n_j^2 - n_j) \right]} \right]^N \quad (6.22)$$

where N is equal to the average number of particles, if one makes an approximation. The approximation consists in fixing the number of cells in the system equal to the average number of particles. This is not to say that the number of particles is fixed. Since the largest contribution to Z_g should be made by terms corresponding to a number of particles not too different from N the approximation should have some value. The chemical potential can be obtained from eq. (6.22) using the relation

$$\langle\langle N \rangle\rangle = \frac{\partial}{\partial \left(\frac{1}{\theta} \mu\right)} \ln Z_g$$

that is

$$\langle\langle N \rangle\rangle = N \frac{1}{Z_g} \sum_{n_g=0}^{\infty} \left[n_j e^{-\frac{1}{\theta} \left[(6K-\mu)n_j + \frac{\rho U_0}{2} (n_j^2 - n_j) \right]} \right]$$

but $N = \langle\langle N \rangle\rangle$ therefore

$$Z_g = \sum_{n_j=0}^{\infty} n_j e^{-\frac{1}{\theta} \left[(6K-\mu)n_j + \frac{\rho U_0}{2} (n_j^2 - n_j) \right]}$$

For $\theta \ll \rho U_0$ one only needs to consider the first three terms in the

infinite sum.

So

$$1 + e^{-\frac{1}{\theta}[(6K-\mu)]} - \frac{1}{\theta}[(6K-\mu)2 + \rho U_0] + e^{-\frac{1}{\theta}[(6K-\mu)2 + \rho U_0]} - \frac{1}{\theta}[(6K-\mu)3 + 3\rho U_0] + e^{-\frac{1}{\theta}[(6K-\mu)3 + 3\rho U_0]} - \frac{1}{\theta}[(6K-\mu)4 + 6\rho U_0] + \dots$$

or

$$1 = e^{-\frac{1}{\theta}[(6K-\mu)2 + \rho U_0]} - \frac{1}{\theta}[(6K-\mu)3 + 3\rho U_0] + e^{-\frac{1}{\theta}[(6K-\mu)3 + 3\rho U_0]} - \frac{1}{\theta}[(6K-\mu)4 + 6\rho U_0] + \dots$$

since the second term is much smaller than the first term one can write expanding the first term

$$1 = 1 - \frac{1}{\theta}[(6K-\mu)2 + \rho U_0] + 2e^{-\frac{1}{\theta}[(6K-\mu)3 + 3\rho U_0]} - \frac{1}{\theta}[(6K-\mu)4 + 6\rho U_0] + \dots$$

so

$$\mu = 6K + \frac{1}{2}\rho U_0 - \theta e^{-\frac{1}{\theta}[\frac{3}{2}\rho U_0]} \quad (6.23)$$

and the assumption that one only needed to consider the first three terms of the infinite sum is proved to be correct.

The values of γ and μ given by equations (6.23) and (6.20) are now known for $x = 0$.

The quantity $n^2 - n$ will now be evaluated for $x = 0$.

From equations (6.12) and (6.13) it follows that:

$$\langle\langle n^2 - n \rangle\rangle = \frac{(r_0)^3}{(2\pi)^4} (-i) \int \frac{G_2(k, \omega - i) - G_2(k, \omega + i)}{\frac{\omega}{\theta} - 1} d^3k d\omega \quad (6.24)$$

From equations (6.10) and (6.10a) it follows that for $x = 0$:

$$G_2(k, \omega) = \frac{2[\omega - (6K - \mu)] + K\gamma}{\rho U_0 \sqrt{1 + 2x\gamma}}. \quad (6.25)$$

$$\left(\frac{1}{\omega - 6K + \mu - \frac{1}{2} \rho U_0 (1 + \sqrt{1 + 2x\gamma})} - \frac{1}{\omega - 6K + \mu + \frac{1}{2} \rho U_0 (1 - \sqrt{1 + 2x\gamma})} \right)$$

Therefore

$$\begin{aligned} \langle\langle n^2 - n \rangle\rangle = \frac{1}{\sqrt{1 + 2x\gamma}} & \left[\left(2 + \frac{3}{2} x\gamma \right) e^{-\frac{6K - \mu + \frac{1}{2} \rho U_0 (1 + \sqrt{1 + 2x\gamma})}{\theta}} - \right. \\ & \left. - \frac{1}{2} x\gamma \left(1 + e^{-\frac{6K - \mu + \frac{1}{2} \rho U_0 (1 - \sqrt{1 + 2x\gamma})}{\theta}} \right) \right] \quad (6.26) \end{aligned}$$

Substituting the expression for $x\gamma$ from equation (6.20) into the previous equation one gets:

$$\langle\langle n^2 - n \rangle\rangle \simeq e^{-\frac{6K - \mu + \frac{1}{2} \rho U_0 (1 + \sqrt{1 + x\gamma})}{\theta}} \quad (6.27)$$

as $\theta \rightarrow 0$ $x\gamma \rightarrow 0$

So

$$\langle\langle n^2 - n \rangle\rangle \rightarrow e^{-\frac{(6K - \mu + \rho U_0)}{\theta}} \quad \text{as } \theta \rightarrow 0 \quad (6.28)$$

with $\mu = 6K + \frac{\rho U_0}{2}$.

After this brief example the question posed about the validity of the two types of approximations will now be answered. The first type of

approximation (letting G_2 be the products of G_1 's is asymptotically exact as $x \rightarrow 0$ independent of the value of T . So, due to the first type of approximation the description is only approximately correct for x "small." The second type of approximation (setting a G_3 equal to G_1 times a number) becomes asymptotically correct only as $x \rightarrow 0$ and $T \rightarrow 0$. For $\theta \ll \rho U_0$ and x "small," G_3 is of very small consequence and so the approximation is valid; however if $\theta \sim \rho U_0$ or larger for any value of x , or if x is not "small" for any value of θ then G_3 becomes important, i.e. the large set of coupled differential equations cannot be done away with, and the approximation for G_3 is no longer appropriate. It follows there that the description of the system will only be valid for x small and $0 \leq \theta \ll \rho U_0$.

Failure to satisfy the equation $\langle\langle n_j \rangle\rangle = 1 = \left(\frac{r_0}{2\pi}\right)^3 \int \langle\langle |a_k^+ a_k| \rangle\rangle d^3k$ is a measure of the error introduced into the description of the system by the approximations made. The equation should, and is, satisfied exactly for $x = 0$, $T = 0$, since the approximations become exact then. How should γ be chosen? The most reasonable way seems to be the choice of γ to satisfy the equation $\langle\langle n_j \rangle\rangle = 1$ in as much as possible, so that γ would be cancelling the effect of every approximation made in as much as a single parameter may. That is how γ was determined for $x = 0$ in equation (6.24). An additional equation must be used to determine μ . This equation will be equivalent to the maximization of Z_g with respect to γ with equation $\langle\langle n_j \rangle\rangle = 1$ as a constraint.

In general, for any x and θ :

$$\begin{aligned}
\langle\langle a_k^+(t) a_k(t) \rangle\rangle &= \frac{1}{2} \frac{1}{\frac{\omega_+ - \mu}{\theta} - 1} + \frac{1}{2} \frac{1}{\frac{\omega_- - \mu}{\theta} - 1} \\
&+ \frac{\frac{3}{2} \rho U_0 - K \sum \cos k \cdot r_0}{(\omega_+ - \omega_-) e^{\frac{\omega_+ - \mu}{\theta}} - 1} - \frac{\frac{3}{2} \rho U_0 - K \sum \cos k \cdot r_0}{(\omega_+ - \omega_-) e^{\frac{\omega_- - \mu}{\theta}} - 1}
\end{aligned} \quad (6.30)$$

follows immediately from equations (6.9) and (6.11). It is then obvious that $\omega_-(k=0) < \mu < \omega_+(k=0)$, otherwise $\langle\langle |a_k^+|^2 \rangle\rangle$ would go to infinity as k approached some value different from zero.

Calculation of Energy and Specific Heat

for $x \ll x_0$ and $\theta \ll x \rho U_0$

The first quantity to be calculated is γ as a function of x and θ . It will then be possible to calculate the energy, E ,

$$E = N6K - NK \sum_{r^i} \langle\langle b_{r_j}^+ b_{r_j+r^i} \rangle\rangle + \frac{N}{2} \rho U_0 \langle\langle n^2 - n \rangle\rangle \quad (6.31)$$

$$h = \sum_{r^i} \langle\langle b_{r_j}^+ b_{r_j+r^i} \rangle\rangle .$$

by computing h and $\langle\langle n^2 - n \rangle\rangle$ separately.

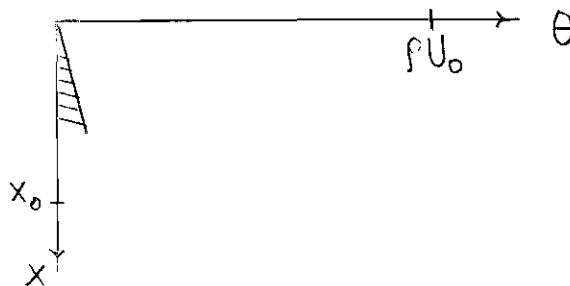


Figure 11. The Results of this Section are Valid Only in the Shaded Area.

It may be well to mention that the results obtained in this section will not be valid at $x = 0$ for $\theta \neq 0$, remember the calculation is only valid for $\theta \ll x\rho U_0$, so that C_v will be obtained for $x \neq 0$ but not for $x = 0$. A different type of approximation would have to be made to obtain the result. But $E(x=0, \theta \neq 0)$ has already been obtained. From equation (6.24) and (6.31) it follows that

$$E(x=0, \theta) = N \left(6K + \frac{\rho U_0}{2} e^{-\frac{1}{2} \frac{\rho U_0}{2\theta}} \right)$$

$$C_v(x=0, \theta) = \frac{1}{2} N \left(\frac{\rho U_0 (\rho U_0)}{2\theta^2} e^{-\frac{1}{2} \frac{\rho U_0}{2\theta}} \right)$$

So, now on with the computation of γ .

$$\langle\langle n_j \rangle\rangle = 1 = \frac{(r_0)^3}{(2\pi)^3} \int \langle\langle |a_k^+ a_k| \rangle\rangle d^3k \text{ determines } \gamma.$$

$\langle\langle |a_k^+ a_k| \rangle\rangle$ is given by equation (6.30).

$$\text{Set } f_1(k) = \frac{1}{2} \frac{1}{\frac{\omega_+ - \mu}{\theta} - 1}; \quad f_2(k) = \frac{1}{2} \frac{1}{\frac{\omega_- - \mu}{\theta} - 1} \quad (6.34)$$

$$f_3(k) = \frac{\frac{3}{2} \rho U_0 - K \sum \cos k \cdot r_0}{(\omega_+ - \omega_-) e^{\frac{\omega_+ - \mu}{\theta}} - 1}; \quad f_4(k) = \frac{\frac{3}{2} \rho U_0 - \sum k \cos k \cdot r_0}{(\omega_+ - \omega_-) e^{\frac{\omega_- - \mu}{\theta}} - 1}$$

$$\langle\langle |a_k^+ a_k| \rangle\rangle = f_1(k) + f_2(k) + f_3(k) + f_4(k). \quad (6.34a)$$

A series expansion is made of these functions now:

$$\frac{1}{\omega_+ - \omega_-} = \frac{1}{\rho U_0} \left[(1 + 3x \cos \mathbf{k} \cdot \mathbf{r}_0 - \alpha - \frac{x^2}{2} (\sum \cos \mathbf{k} \cdot \mathbf{r}_0)^2 + \right. \\ \left. + \frac{3}{8} 36x^2 (\sum \cos \mathbf{k} \cdot \mathbf{r}_0)^2 - 24\alpha [\cos \mathbf{k} \cdot \mathbf{r}_0 + 4x^2 \gamma^2 + \dots +]) \right]$$

where $x = x\gamma$.

Correct to order x^2 and $x(x\gamma)$

let $\omega_+(k) - \mu = \omega_+(k) - \omega_+(0) + (\omega_+(0) - \mu)$; let $f(\theta, x) = \omega_+(0) - \mu$

$\omega_-(k) - \mu = \omega_-(k) - \omega_-(0) + (\omega_-(0) - \mu)$ and $g(\theta, x) = \mu - \omega_-(0)$

as it was shown previously $g(x, \theta) > 0$ and $f(\theta, x) > 0$ exactly what values g and f will have may be determined by the equation

$$1 = \langle n_j \rangle \quad g(\theta, x) + f(\theta, x) = \omega_+(0) - \omega_-(0)$$

Making use of (6.11a) expanded in series, one obtains:

$$\omega_+(k) - \mu = f(\theta, x) + \frac{1}{2} \rho U_0 \left[-4x \sum_{\mathbf{r}_0} \cos \bar{\mathbf{k}} \cdot \bar{\mathbf{r}}_0 + 12x - \right. \\ \left. - 4x^2 \sum_{\mathbf{r}_0} \cos \mathbf{k} \cdot \mathbf{r}_0^2 + 36x^2 + 3x\alpha \sum \cos \bar{\mathbf{k}} \cdot \bar{\mathbf{r}}_0 - 9x\alpha \right] \\ \omega_-(k) - \mu = -g(\theta, x) - \frac{1}{2} \rho U_0 \left[-2x \sum_{\mathbf{r}_0} \cos \bar{\mathbf{k}} \cdot \mathbf{r}_0 + 6x - \right. \\ \left. - 4x^2 \sum_{\mathbf{r}_0} \cos \bar{\mathbf{k}} \cdot \bar{\mathbf{r}}_0^2 + 36x^2 + 3x\alpha \sum \cos \bar{\mathbf{k}} \cdot \bar{\mathbf{r}}_0 - 9x\alpha \right] \quad (6.37)$$

Making use of equations (6.34) and (6.35) one can obtain:

$$f_1(k) = \frac{1}{2} \left(e^{-\frac{\omega_+ - \mu}{\theta}} + e^{-2\frac{\omega_+ - \mu}{\theta}} + \dots \right); f_2(k) = -\frac{1}{2} \left(1 + e^{\frac{\omega_- - \mu}{\theta}} + e^{2\frac{\omega_- - \mu}{\theta}} + \dots \right) \quad (6.38)$$

$$\begin{aligned}
f_3(k) = & \left(\frac{3}{2} \rho U_0 - K \sum_{\vec{r}_0} \cos \vec{k} \cdot \vec{r}_0 \right) \frac{1}{\rho U_0} \left(1 + 3x \sum_{\vec{r}_0} \cos \vec{k} \cdot \vec{r}_0 - x\gamma + \right. \\
& + 13x^2 \left(\sum_{\vec{r}_0} \cos \vec{k} \cdot \vec{r}_0 \right)^2 - 9x\gamma \sum_{\vec{r}_0} \cos \vec{k} \cdot \vec{r}_0 + \frac{3}{2} x^2 \gamma^2 \left. \right) \left(e^{-\frac{\omega_+ - \mu}{\theta}} + \right. \\
& \left. + e^{-2\frac{\omega_+ - \mu}{\theta}} + \dots \right) \quad (6.39)
\end{aligned}$$

$$\begin{aligned}
f_4(k) = & \left(\frac{3}{2} \rho U_0 - K \sum_{\vec{r}_0} \cos \vec{k} \cdot \vec{r}_0 \right) \frac{1}{\rho U_0} \left(1 + 3x \sum_{\vec{r}_0} \cos \vec{k} \cdot \vec{r}_0 - x\gamma + \right. \\
& + 13x^2 \sum_{\vec{r}_0} \cos \vec{k} \cdot \vec{r}_0^2 - 9x^2 \gamma \sum_{\vec{r}_0} \cos \vec{k} \cdot \vec{r}_0 + \frac{3}{2} x^2 \gamma^2 \left. \right) \left(1 + e^{\frac{\omega_- - \mu}{\theta}} + \right. \\
& \left. + 2 \frac{2(\omega_- - \mu)}{\theta} + \dots \right) \quad (6.40)
\end{aligned}$$

Now for

$$\begin{aligned}
x \ll x_0 \quad \omega_+(0) - \omega_-(0) & \simeq \rho U_0 \\
& = f(\theta, x) + g(\theta, x)
\end{aligned}$$

also $f(\theta, x) > 0$, $g(\theta, x) > 0$

It follows from equations (6.30) that the smaller either $\omega_+(0) - \mu$ or $\mu - \omega_-(0)$ is the larger $\langle\langle |a_{k=0}^* a_{k=0}| \rangle\rangle$ is. For either $\omega_+(0) - \mu = 0$ or $\mu - \omega_-(0) = 0$ $\langle\langle |a_k^* a_k| \rangle\rangle = \infty$ therefore $g(\theta, x)$ and $f(\theta, x)$ must be of the same order of magnitude for $x \ll x_0$ and $\theta \ll x \rho U_0$. It will be assumed, then, that the series of exponentials in equations (6.38), (6.39) and (6.40) are rapidly converging. Therefore

$$f_1(k) \simeq \frac{1}{2} e^{-\frac{\omega_+ - \mu}{\theta}}; \quad f_2(k) = -\frac{1}{2} \left(1 + e^{\frac{\omega_- - \mu}{\theta}} \right) \quad (6.42)$$

$$f_3(k) \simeq \left(\frac{3}{2} \rho U_0 - K \int_{r_0} \cos \bar{k} \cdot \bar{r}_0 \right) \frac{1}{\rho U_0} \left(1 + 3x \int_{r_0} \cos \bar{k} \cdot \bar{r}_0 - \right. \\ \left. - x\gamma + 13x^2 \int_{r_0} \cos \bar{k} \cdot \bar{r}_0^2 - 9x^2 \gamma \int_{r_0} \cos \bar{k} \cdot \bar{r}_0 + \frac{3}{2} x^2 \gamma^2 \right) e^{-\frac{\omega_+ - \mu}{\theta}} \quad (6.43)$$

$$f_4(k) = \left(\frac{3}{2} \rho U_0 - K \int_{r_0} \cos \bar{k} \cdot \bar{r}_0 \right) \frac{1}{\rho U_0} \left(1 + 3x \int_{r_0} \cos \bar{k} \cdot \bar{r}_0 - x\gamma + \right. \\ \left. + 13x^2 \int_{r_0} \cos \bar{k} \cdot \bar{r}_0^2 - 9x^2 \gamma \int_{r_0} \cos \bar{k} \cdot \bar{r}_0 + \frac{3}{2} x^2 \gamma^2 \right) 1 + e^{-\frac{\omega_- - \mu}{\theta}} \quad (6.44)$$

$x\gamma$ will now be evaluated making use of equations (6.16) and (6.34a).

$$\langle\langle n_j \rangle\rangle = \frac{(r_0)^3}{(2\pi)^3} \int \left[-\frac{1}{2} + \frac{3}{2} \left(1 - \frac{x}{3} \int \cos k r_0 \right) \left(1 + 3x \int \cos k \cdot r_0 - \right. \right. \\ \left. \left. - x\gamma + 13x^2 \int \cos k r_0^2 - 9x\gamma \int \cos k r_0 + \frac{3}{2} x^2 \gamma^2 \right) \right] 4\pi k^2 dk \\ + \frac{(r_0)^3}{(2\pi)^3} \int \left[\left(\frac{1}{2} + \frac{3}{2} \right) e^{-\frac{f}{\theta}} e^{-\frac{1}{2} \frac{\rho U_0}{\theta} x^2 (k \cdot r_0)^2} + \right. \\ \left. \left(-\frac{1}{2} + \frac{3}{2} \right) e^{-\frac{g}{\theta}} e^{-\frac{1}{2} \frac{\rho U_0}{\theta} x (k \cdot r_0)^2} \right] d^3 k \quad 4\pi k^2$$

The lower limit of integration is zero, the upper limit is such that

$$1 = \left(\frac{r_0}{2\pi} \right) \int_0^a 4\pi k^2 dk ;$$

is satisfied

$$\text{So} \quad a = 3 \sqrt{\frac{3}{4\pi}} \left(\frac{2\pi}{r_0} \right)$$

the equation (45) is correct to order x^2 and $e^{-\frac{f}{\theta}}$, not to order $x^2 e^{-\frac{f}{\theta}}$, not to order $e^{-2\frac{f}{\theta}}$ or $e^{-2\frac{g}{\theta}}$

$$n_j = 1 - \frac{3}{2} x\gamma + \frac{3}{2} 18x^2 + \left(\frac{3}{2}\right)^2 x^2 \gamma^2 + \frac{g}{2} x^3 \gamma \frac{3}{2} + \frac{\sqrt{\pi}}{8\pi^2} \frac{\theta}{\rho U_o x}^{3/2} e^{-\frac{f}{\theta}} + \frac{\sqrt{\pi}}{8\pi^2} \frac{2\theta}{\rho U_o x}^{3/2} e^{-\frac{g}{\theta}} \quad (6.46)$$

this result was obtained from equation (45) using the fact that $\frac{\theta}{\rho U_o x} \ll 1$.

It follows from the last equation that:

$$x\gamma = 18x^2 + \frac{\sqrt{\pi}}{12\pi^2} \left(\frac{\theta}{\rho U_o x}\right)^{3/2} e^{-\frac{f}{\theta}} + \frac{\sqrt{2}}{6} \frac{\sqrt{\pi}}{\pi^2} \left(\frac{\theta}{\rho U_o x}\right)^{3/2} e^{-\frac{g}{\theta}} \quad (6.47)$$

For $x \ll x_o$ and $\theta \ll x\rho U_o$.

Again only one equation is obtained relating γ and μ . Another equation can be written to obtain γ , and that is

$$\frac{\partial \ln Zg}{\partial \gamma} = 0$$

Zg was previously obtained in an approximate form for $x = 0$. It is necessary now to have Zg for $x \neq 0$ to obtain γ from the previous equation.

Let H , the Hamiltonian for the system be given by $H = H_o + \lambda V$, where λV is the perturbing part.

$$Zg = \text{trace } e^{-\frac{1}{\theta} [H_o + \lambda V - \mu N]}$$

$$\frac{\partial}{\partial \lambda} \ln Zg = \frac{\text{trace } (-\frac{1}{\theta}) V e^{-\frac{1}{\theta}[H_0 + \lambda V - \mu N]}}{\text{trace } e^{-\frac{1}{\theta}[H_0 + \lambda V - \mu N]}}$$

that is

$$\frac{\partial \ln Zg}{\partial \lambda} = -\frac{1}{\theta} \langle\langle V \rangle\rangle$$

and

$$\ln Z_{\lambda=1} = \ln Zg_{\lambda=0} + \int_{\lambda=0}^{\lambda=1} (-\frac{1}{\theta}) \langle\langle V \rangle\rangle_{\lambda} d\lambda \quad (6.49)$$

Now in the case treated here

$$H_0 = 6K \sum_{r_j} b_{r_j}^* b_{r_j} + \frac{\rho U_0}{2} \sum_{r_j} b_{r_j}^* b_{r_j}^* b_{r_j} b_{r_j} \quad \text{and} \quad \lambda V = -\lambda K \sum_{r_j, r'} b_{r_j}^* b_{r_j+r'}.$$

From equation (6.50) one can write

$$\begin{aligned} \langle\langle V \rangle\rangle_{\lambda} = & \frac{(r_0)^3}{(2\pi)^3} \int \left[-\frac{1}{2} + \frac{3}{2} \left(1 - \frac{\lambda x}{3} \sum_{r_0} \cos k \cdot r_0 \right) (1 + 3\lambda x \sum_{r_0} \cos k \cdot r_0 - \right. \\ & - \lambda x \gamma + 13\lambda^2 x^2 \sum_{r_0} \cos k \cdot r_0^2 + \frac{3}{2} \lambda^2 \gamma^2 - \\ & - 9\lambda^3 x^3 \gamma \sum_{r_0} \cos k r_0^2 \sum_{r_0} \cos k r_0^2 4\pi^2 k^2 dk) \left. \right] 4\pi^2 k^2 dk \\ & + \left(\frac{r_0}{2\pi} \right)^3 \int \left[\left(\frac{1}{2} + \frac{3}{2} \right) e^{-\frac{f}{\theta}} e^{-\frac{1}{2} \frac{\rho U_0}{e}} dx \rho (k r_0)^2 + \right. \\ & + \left. \left(-\frac{1}{2} + \frac{3}{2} \right) e^{-\frac{g}{\theta}} e^{-\frac{1}{2} \frac{\rho U_0}{\theta}} (x(k r_0)^2) \right] 2 \sum_{r_0} \cos k r_0^2 4\pi k^2 dk \quad (6.49a) \end{aligned}$$

The grand-canonical partition function must be maximized with respect to γ with the constraint that the average number of particles per cell should be one, i.e. the integral $\int_{\lambda=0}^{\lambda=1} h_{\lambda} d\lambda$ must be minimized with respect to γ with equation (6.47) as a constraint.

Let

$$g_{\lambda}(\gamma, \mu) = x\gamma - 18x^2 - \frac{\sqrt{\pi}}{12\pi^2} \left(\frac{\theta}{\rho U_0 x} \right)^{3/2} e^{-\frac{f}{\theta}} - \frac{\sqrt{2}}{6} \frac{\sqrt{\pi}}{\pi^2} \frac{\theta}{(\rho U_0 x)} e^{-\frac{g}{\theta}}$$

where $g = \mu - \omega_{-}(0)$ and $f = \omega_{+}(0) - \mu$.

The equations to be solved to satisfy the minimization condition are

$$\frac{\partial \langle V_{\lambda} \rangle}{\partial \mu} + \lambda \frac{\partial g}{\partial \mu} = 0$$

$$\frac{\partial \langle V_{\lambda} \rangle}{\partial \gamma} + \lambda \frac{\partial g}{\partial \gamma} = 0$$

$$g_{\lambda}(\mu, \gamma) = 0$$

From equations (6.49a) and (6.47) it follows that the previous equations may be written as

$$-\frac{3}{4} e^{-\frac{f}{\theta}} - \sqrt{2} \frac{3}{2} e^{-\frac{g}{\theta}} - \lambda \frac{1}{12} e^{-\frac{f}{\theta}} + \lambda \frac{\sqrt{2}}{6} e^{-\frac{g}{\theta}} = 0$$

$$-\frac{3}{2} x^2 + \left(\frac{3}{2}\right)^2 x^3 \gamma + \lambda x = 0$$

$$g(\gamma, \mu) = 0$$

One can rewrite the first of these three equations as

$$+ \frac{3}{4} e^{-\frac{f}{\theta}} - \sqrt{2} \frac{3}{2} e^{-\frac{g}{\theta}} + \lambda \frac{1}{9} \left(-\frac{3}{4} e^{-\frac{f}{\theta}} + \sqrt{2} \frac{3}{2} e^{-\frac{g}{\theta}} \right) = 0$$

The previous equation is satisfied if

$$\frac{3}{4} e^{-\frac{f}{\theta}} = \sqrt{2} \frac{3}{2} e^{-\frac{g}{\theta}}$$

These relations are correct for $\theta \ll x\rho U_0$ and $x \ll x_0$, i.e.

$\omega_+(0) - \omega_-(0) \gg \theta$, but $f + g = \omega_+(0) - \omega_-(0)$, therefore the previous equation is satisfied if g is slightly larger than f , i.e.

$\mu = \frac{\omega_+(0) + \omega_-(0)}{2}$ for $x \ll x_0$ and $x\rho U_0 \gg \theta$. The value for γ is now given by equation (6.47). Values for μ and γ have been obtained previously for $x = 0$. In the next section μ and γ will be obtained for $x = x_0$.

Now $h = \sum \langle \langle b_{r_j}^* b_{r_j+r_0} \rangle \rangle$ will be computed.

$$\begin{aligned} h = & \left(\frac{r_0}{2\pi}\right)^3 \int \left[-\frac{1}{2} + \frac{3}{2} \left(1 - \frac{x}{3} \sum \cos k \cdot r_0\right) \left(1 + 3x \sum \cos k \cdot r_0 - \right. \right. \\ & \left. \left. - x\gamma + 12x^2 \sum \cos k r_0^2 + \frac{3}{2} x^2 \gamma^2 - \right. \right. \\ & \left. \left. - 9x^3 \gamma (\cos k r_0)^2 \sum \cos k r_0\right) 4\pi k^2 dk \right] + \\ & + \left(\frac{r_0}{2\pi}\right)^3 \int \left[\left(\frac{1}{2} + \frac{3}{2}\right) e^{-\frac{f}{\theta}} e^{-\frac{1}{2} \frac{\rho U_0}{\theta} x 2(kr_0)^2} + \right. \\ & \left. + \left(-\frac{1}{2} + \frac{3}{2}\right) e^{-\frac{g}{\theta}} e^{-\frac{1}{2} \frac{\rho U_0}{\theta} x (kr_0)^2} \right] 2 \sum \cos k r_0 4\pi k^2 dk \quad (6.50) \end{aligned}$$

In the second integral let $2 \int \cos kr_0 = 6$ since $e^{-\frac{1}{2} \frac{\rho U_0 x}{\theta} (kr_0)^2}$ is a very fast decreasing function of k and it goes to zero very rapidly as k **departs** from zero. It is well known that

$$\int_0^a e^{-bx^2} x^2 dx \rightarrow \int_0^\infty e^{-bx^2} x^2 dx$$

for any $a > 0$ as $b \rightarrow \infty$, so the approximation for $2 \int \cos kr_0$ is valid.

$$h = 12x + \frac{3}{4} \frac{\sqrt{\pi}}{\pi^2} \left(\frac{\theta}{\rho U_0 x} \right)^{3/2} e^{-\frac{f}{\theta}} + \frac{\sqrt{2} \cdot 3}{2} \frac{\sqrt{\pi}}{\pi^2} \left(\frac{\theta}{\rho U_0 x} \right)^{3/2} e^{-\frac{g}{\theta}} \quad \text{for } x \ll x_0$$

and $\theta \ll \rho U_0 x$

with $g = f = \frac{\omega_+(0) - \omega_-(0)}{2}$

From equations (6.10)(6.12) and (6.13) it follows that

$$\begin{aligned} \langle\langle n^2 - n \rangle\rangle &= \left(\frac{r_0}{2\pi} \right)^3 \int g(k) d^3k \quad \text{and} \quad g(k) = \frac{1}{\frac{\omega_+ - \mu}{\theta} - 1} + \frac{1}{\frac{\omega_- - \mu}{\theta} - 1} + \\ &+ \frac{2(\frac{1}{2} \rho U_0 - K \sum \cos kr_0) + K\gamma}{(\omega_+ - \omega_-) \frac{\omega_+ - \mu}{\theta} - 1} - \frac{2(\frac{1}{2} \rho U_0 - K \sum \cos kr_0) + K\gamma}{(\omega_+ - \omega_-) \frac{\omega_- - \mu}{\theta} - 1} \end{aligned} \quad (6.52)$$

let

$$\begin{aligned} e_1(k) &= \frac{1}{\frac{\omega_+ - \mu}{\theta} - 1} & e_2(k) &= \frac{1}{\frac{\omega_- - \mu}{\theta} - 1} \\ e_3(k) &= \frac{2(\frac{1}{2} \rho U_0 - K \sum) + K\gamma}{(\omega_+ - \omega_-) \frac{\omega_+ - \mu}{\theta} - 1} & e_4(k) &= \frac{2(\frac{1}{2} \rho U_0 - k \sum) + K\gamma}{(\omega_+ - \omega_-) \frac{\omega_- - \mu}{\theta} - 1} \end{aligned} \quad (6.53)$$

$$e_1 = e^{-\frac{\omega_+ - \mu}{\theta}} + \dots$$

$$e_2 = -1 - e^{\frac{\omega_- - \mu}{\theta}} + \dots$$

$$e_3 = \frac{2(\frac{1}{2}\rho U_0 - K \int \cos kr_0) + K\gamma}{\rho U_0} (1 + 3x \int \cos kr_0 - x +$$

$$+ 13x^2 \int \cos^2 kr_0 - 9x^2 \int \cos kr_0 + \frac{3}{2} x^2 \gamma^2) e^{-\frac{\omega_+ - \mu}{\theta}}$$

$$e_4 = \frac{2(\frac{1}{2}\rho U_0 - K \int \cos kr_0) + K\gamma}{\rho U_0} (1 + 3x \int \cos kr_0 - x +$$

$$+ 12x^2 \int \cos^2 kr_0 - 9x^2 \int \cos kr_0 + \frac{3}{2} x^2 \gamma^2) 1 + e^{\frac{\omega_- - \mu}{\theta}} \quad (6.54)$$

$$\langle\langle n^2 - n \rangle\rangle = \frac{(r_0)^3}{(2\pi)^3} \int [-1 + (1 - x \int \cos kr_0 + \frac{\gamma x}{2})(1 + 3x \cos kr_0 -$$

$$- x\gamma + 13x^2 \int \cos^2 kr_0 - 9x\gamma \int \cos kr_0 + 3x^2 \gamma^2)] 4\pi k^2 dk$$

$$+ \int [-1 + (1 - x \int \cos kr_0 + \frac{x}{2} \gamma)(1 + 3x \int \cos kr_0 - x\gamma +$$

$$+ 13x^2 \int \cos^2 kr_0 - 9x^2 \gamma \int \cos kr_0 + 3x^2 \gamma^2)] e^{\frac{\omega_- - \mu}{\theta}} 4\pi k^2 dk$$

$$+ \int [1 + (1 - x \int \cos kr_0 + \frac{x}{2} \gamma)(1 + 3x \int \cos kr_0 - x\gamma +$$

$$+ 13x^2 \int \cos^2 kr_0 - 9x\gamma^2 \int \cos kr_0 + 3x^2 \gamma^2)] e^{\frac{\omega_+ - \mu}{\theta}} 4\pi k^2 dk$$

$$= x\gamma + \frac{39}{2} x^2 + 3x^2 \gamma^2 - \frac{9}{2} x^2 + \frac{x}{2} \gamma + \frac{\sqrt{\pi}}{8\pi^2} \left(\frac{\theta}{\rho U_0 x}\right)^{3/2} e^{-\frac{f}{\theta}}$$

$$n^2 - n = 6x^2 + \frac{\sqrt{\pi}}{8\pi^2} \left(\frac{\theta}{\rho U_o x}\right)^{3/2} e^{-\frac{f}{\theta}} \quad \text{for } x \ll x_o \quad \theta \ll x \rho U_o \quad (6.55)$$

From equations (6.31), (6.49) and (6.53) one gets:

$$\begin{aligned} E &= N \left[6K - K12x + \frac{1}{2} \rho U_o \left(6x^2 + \frac{\sqrt{\pi}}{8\pi^2} \left(\frac{\theta}{\rho U_o x}\right)^{3/2} e^{-\frac{f}{\theta}} \right) \right] \\ &= N \left[6K - 6K(x) + \rho U_o \left(\frac{\sqrt{\pi}}{(6\pi)^2} \left(\frac{\theta}{\rho U_o x}\right)^{3/2} \right) e^{-\frac{f}{\theta}} \right] \end{aligned} \quad (6.56)$$

$$\begin{aligned} C_v = \frac{\partial E}{\partial T} \bigg|_v &= \frac{\partial E}{\partial \theta} s = s \frac{3}{32} \frac{\sqrt{\pi}}{\pi^2} \left(\frac{\theta}{\rho U_o x}\right)^{\frac{1}{2}} \frac{1}{x} e^{-\frac{f}{\theta}} + s \rho U_o \frac{\pi}{(6\pi)^2} \frac{f}{\theta^2} \left(\frac{\theta}{\rho U_o x}\right)^{\frac{3}{2}} e^{-\frac{f}{\theta}} \\ &\quad + s \rho U_o \frac{\pi}{16\pi^2} \frac{1}{\theta} \frac{\partial f}{\partial \theta} \left(\frac{\theta}{\rho U_o x}\right)^{3/2} e^{-\frac{f}{\theta}} \end{aligned}$$

where s is the Boltzman constant.

The first term is down by a factor of $\frac{\rho U_o}{\theta}$ from the second one so it is neglected. The specific heat is given by:

$$C_v = \frac{1}{16} \frac{\sqrt{\pi}}{\pi^2} k \left[\frac{\rho U_o f(\theta, x)}{\theta^2} \left(\frac{\theta}{\rho U_o x}\right)^{3/2} e^{-\frac{f(\theta, x)}{\theta}} + - \frac{\rho U_o}{\theta} \frac{\partial f}{\partial \theta} \left(\frac{\theta}{\rho U_o x}\right)^{\frac{3}{2}} e^{-\frac{f(\theta, x)}{\theta}} \right]$$

$\frac{\partial f}{\partial \theta}$ is a negative number if $\frac{\partial \mu}{\partial \theta} < 0$.

Density of Instability

It is the purpose of this section to show how the density of the instability in the description of the system changes with temperature.

The results obtained in this section will be valid for $\theta \ll \rho U_o$

due to the approximations previously introduced in the Green functions equations.

The density of instability will be denoted by $\rho_o(T), x_o(T) = \frac{1}{mU_o \rho_o^{1/3}}$ follows from the definition of x .

The instability occurs at a density given by the equation:

$$\omega_+(0) - \omega_-(0) = 0. \quad (6.58)$$

There is only one term in $\omega_+(0) - \omega_-(0)$ which depends on T , therefore ρ_o will depend on T .

The value obtained for $x\gamma$ in equation (6.47) satisfies equation

$$1 = \frac{(r_o)^3}{(2\pi)^3} \int \langle\langle a_k^* a_k \rangle\rangle d^3k$$

for $x \ll x_o$ and $\theta \ll x\rho U_o$.

If one assumes temporarily that the value obtained in (6.47) is valid for $x \leq x_o$ one can then obtain a value of $x_o(T)$ from equation (6.58). Substituting the values of $\omega_+(0) - \omega_-(0)$ from equation (6.10a) into equation (6.58) one gets:

$$(1 - 3x_o)^2 - 12x_o + 2x\gamma = 0 \quad (6.59)$$

Using equation (6.47) one obtains

$$0 = (1 - 3x_o)^2 - 12x_o + 2(18x_o^2) + 2 \left(\frac{\theta}{\rho U_o x} \right)^{\frac{3}{2}} \left(\frac{\sqrt{\pi}}{12\pi^2} \right) \left(e^{-\frac{f(\theta, x)}{\theta}} + e^{-\frac{g(\theta, x)}{\theta}} \right)$$

Now, since $(\frac{\theta}{\rho U_o x}) \ll 1$ one obtains

$$x_o(T) \simeq \frac{6}{90} \left[1 + .8 \frac{\sqrt{\pi}}{\pi^2} \left(\frac{\theta}{\rho U_o x} \right)^{\frac{3}{2}} \right] \quad (6.60)$$

but

$$x_o(T) = \frac{1}{m U_o [\rho(t)]^{3/2}}$$

therefore

$$\rho_o(T) = (15)^3 \frac{1}{(m U_o)^3} \left[1 - \frac{.8 \sqrt{\pi}}{\pi^2} \left(\frac{\theta}{\rho U_o x} \right)^{3/2} \right]^3 \quad (6.60a)$$

$\rho_o(T)$ decreases as T increases, whereas the density of He^4 along the melting line increases as T increases. The significance of this result will be discussed later. An expression for $\rho_o(T)$ will now be obtained without assuming the value of x_T to be given by equation (6.47) at $x = x_o$. This will be done by solving for x_o the equation

$$1 = \frac{(r_o)^3}{(2\pi)^3} \int f_1(k) + f_2(k) + f_3(k) + f_4(k) d^3k \quad \text{with } \omega_+(0) - \omega_-(0) = 0$$

where

$$f_1(k) = \frac{1}{2} e^{-\frac{\omega_- - \mu}{\theta}}$$

$$f_2(k) = -\frac{1}{2} - \frac{1}{2} e^{\frac{\omega_- - \mu}{\theta}} + \dots$$

$$f_3(k) = \frac{\frac{3}{2} \rho U_o - K \sum \cos \vec{k} \cdot \vec{r}_o}{\omega_+ - \omega_-} e^{-\frac{\omega_+ - \mu}{\theta}} + \dots$$

the value of the first integral depends on θ only through $x(\theta)$. It will be shown now that $p_o(\theta)$ decreases as θ increases.

Making a series expansion of $p_o(\theta)$ and $x_o(\theta)$,

$$\begin{aligned} p_o(\theta) &= p_o(0) + \frac{\partial p_o}{\partial \theta} \theta + \frac{1}{2} \frac{\partial^2 p_o}{\partial \theta^2} \theta^2 + \dots \\ x_o(\theta) &= x_o(0) + \frac{\partial x_o}{\partial \theta} \theta + \frac{1}{2} \frac{\partial^2 x_o}{\partial \theta^2} \theta^2 + \dots \end{aligned} \quad (6.65)$$

Every derivative of x_o is related to a derivative of p_o . For the first derivative,

$$\frac{\partial x_o}{\partial \theta} = \frac{\partial x_o}{\partial p_o} \frac{\partial p_o}{\partial \theta} \quad (6.66)$$

but $x = \frac{1}{m_p^{1/3} U_o}$

therefore $\frac{\partial x_o}{\partial \theta} = -\frac{1}{3} \frac{x_o}{p_o} \frac{\partial p_o}{\partial \theta}$

By inspection of equation (6.64) one realizes that the second integral is of order θ^2 and higher powers of θ , therefore in order to satisfy equation (6.64) it is necessary that:

$$\frac{\partial p_o}{\partial \theta} = 0$$

and, of course,

$$\frac{\partial x_o}{\partial \theta} = 0.$$

With this in mind one can write;

$$f_4(k) = \frac{\frac{3}{2} \rho U_0 - k \sum_{\vec{r}_0} \cos \vec{k} \cdot \vec{r}_0}{\omega_+ - \omega_-} \left(1 + e^{\frac{\omega_- - \mu}{\theta}} + \dots \right)$$

Now, from equation (10a) it follows that for $x = x_0$, i.e. $\omega_+(0) - \omega_-(0) = 0$, and $|k| \ll \frac{\pi}{r_0}$,

$$\begin{aligned} \omega_+(k) &= \frac{1}{2} \rho U_0 (1 + 3x_0) + \frac{1}{2} |k| \left[\frac{3\rho U_0 (1 - x_0)}{m} \right]^{1/2} \\ \omega_-(k) &= \frac{1}{2} \rho U_0 (1 + 3x_0) - \frac{1}{2} |k| \left[\frac{3\rho U_0 (1 - x_0)}{m} \right]^{1/2} \end{aligned} \quad (6.61)$$

therefore $\mu = \frac{1}{2} \rho U_0 (1 + 3x_0)$ for $x = x_0$.

Let

$$C = \frac{1}{2\theta} \sqrt{\frac{3(1 - x_0)\rho U_0}{m}}; \quad (6.62)$$

$$\begin{aligned} \omega_+ - \mu &= \theta C |k| \\ \omega_- - \mu &= -\theta C |k| \end{aligned} \quad (6.63)$$

Now

$$\begin{aligned} 1 &= \left(\frac{r_0}{2\pi}\right)^3 \int \left[-\frac{1}{2} + \frac{3}{2} \rho U_0 \left(1 - \frac{x_0}{3}\right) \sum_{\vec{r}_0} \cos \vec{k} \cdot \vec{r}_0 \frac{1}{2\theta C |k|} \right] d^3k + \\ &+ \int \frac{3}{2} \rho U_0 (1 - x_0) \sum_{\vec{r}_0} \cos \vec{k} \cdot \vec{r}_0 \frac{2e^{-Ck}}{2\theta |k|} d^3k. \end{aligned}$$

Obviously, the second integral in the previous expression is larger than zero for $\theta \neq 0$, and it vanishes at $\theta = 0$. It follows, therefore, that the value of the first integral must decrease as θ increases, but

$$\frac{\partial^2 x_o}{\partial \theta^2} = -\frac{1}{3} \frac{x_o}{\rho_o} \frac{\partial^2 \rho_o}{\partial \theta^2}$$

So one can now write equation (6.65) as

$$\begin{aligned} \rho_o(\theta) &= \rho_o(0) + \frac{1}{2} \frac{\partial^2 \rho_o}{\partial \theta^2} \theta^2 + \dots \\ x_o(\theta) &= x(0) + \frac{1}{6} \frac{x_o}{\rho_o} \frac{\partial^2 \rho_o}{\partial \theta^2} \theta^2 \end{aligned} \quad (6.67)$$

An expression appearing in equation (6.64) can now be written as follows:

$$\begin{aligned} \frac{\frac{3}{2} \rho_o U_o (1 - \frac{x}{3} \sum_{\vec{r}_o} \cos \vec{k} \cdot \vec{r}_o)}{2 C \theta |k|} &= \frac{\frac{3}{2} U_o (\sqrt{\rho_o(0)} + \frac{1}{4} \frac{1}{\sqrt{\rho_o(0)}} \frac{\partial^2 \rho_o}{\partial \theta^2} \theta^2)}{|k| \sqrt{\frac{3U_o}{m}}} \\ &[1 - \frac{1}{3} \sum_{\vec{r}_o} \cos \vec{k} \cdot \vec{r}_o ((x_o(0) - \frac{1}{6} \frac{x_o(0)}{\rho_o(0)} \frac{\partial^2 \rho_o}{\partial \theta^2} \theta^2)) [1 + \frac{1}{2} (x_o(0) - \\ &- \frac{1}{6} \frac{x_o(0)}{\rho_o(0)} \frac{\partial^2 \rho_o}{\partial \theta^2} \theta^2 + \dots)] \quad (6.68) \end{aligned}$$

Equation (6.64) may be rewritten now considering only the leading terms in equation (6.68):

$$\begin{aligned} 1 &= \left(\frac{r_o}{2\pi}\right)^3 \int \left[-\frac{1}{2} + \frac{3}{2} \rho_o U_o \left(1 - \frac{x(0)}{3} \sum \cos \vec{k} \cdot \vec{r}_o\right) \frac{1}{2 \theta C(t) |k|}\right] d^3 k + \\ &+ \frac{1}{4} \frac{1}{\rho(0)} \frac{\partial^2 \rho}{\partial \theta^2} \theta^2 \int \frac{3}{2} \rho_o U_o \left(1 - \frac{x(0)}{3} \sum \cos \vec{k} \cdot \vec{r}_o\right) \frac{1}{2 \theta C(0) |k|} d^3 k + \end{aligned}$$

$$+ \int \frac{3}{2} p(0) U_0 \left(1 - \frac{x(0)}{3} \sum \cos kr_0\right) \frac{2e^{-C|k|}}{2\theta C(0)|k|} d^3k \quad (6.69)$$

It is clear that the second term must cancel the third term since the first term is equal to u_j at $\theta = 0$. This cancellation can only occur if $\frac{\partial^2 p}{\partial \theta^2} < 0$.

$$\frac{\partial^2 p}{\partial \theta^2} = - \frac{4p(0)}{\theta^2} \frac{\int \left(1 - \frac{x(0)}{3} \sum \cos kr_0\right) \frac{2e^{-C|k|}}{2\theta C(0)|k|} d^3k}{\int \left(1 - \frac{x(0)}{3} \sum \cos kr_0\right) \frac{1}{2\theta C(0)|k|} d^3k} \quad (6.70)$$

This calculation is somewhat rough, only the first two terms in the expansion of p and x were considered, and already the terms in $\frac{\partial^2 p}{\partial \theta^2}$ down by a factor of x were neglected. The two terms down by a factor of x in the previous expression will be neglected to get:

$$\frac{\partial^2 p}{\partial \theta^2} = - \frac{4p(0)}{\theta^2} \frac{\int \frac{2e^{-C|k|}}{2\theta C(0)|k|} d^3k}{\int \frac{1}{2\theta C(0)|k|} d^3k} \quad (6.71)$$

$$\int \frac{2e^{-C|k|}}{2\theta C(0)|k|} 4\pi k^2 dk \simeq 32\pi \left(\frac{m}{3\rho U_0}\right)^{3/2} \theta^2 \quad (6.72)$$

$$\int_0^{k=(\frac{2\pi}{r_0})^3 \sqrt{\frac{3}{4\pi}}} \frac{1}{2\theta C(0)|k|} 4\pi k^2 dk = \frac{4\pi}{2} \left(\frac{2\pi}{r_0}\right)^2 \left(\frac{3}{4\pi}\right)^{2/3} \sqrt{\frac{m}{3\rho U_0}}; \frac{1}{r_0^2} = 2mK \quad (6.73)$$

so

$$p_0(\theta) \simeq p_0(0) - \frac{1,2}{x_0(0)} \frac{1}{\rho_0(0)U_0^2} \theta^2$$

or equivalently,

$$\rho_o(\theta) \simeq \rho_o(0) - \frac{m}{\hbar^2 2/3 \mu_o} \theta^2 \quad (6.74)$$

This result differs from the one obtained previously in equation (6.60a). This should not be surprising because the value of $x_o(\theta)$ given in equation (6.60a) was obtained using a value of γ which was valid for $x \ll x_o$ only; therefore that result was expected to have a qualitative significance but not quantitative. The most significant feature of the result is the negative sign of the second derivative of $\rho_o(\theta)$ with respect to θ . The density of instability is a decreasing function of temperature. On the other hand, the density along the melting line of He^4 is an increasing function of temperature. What is, then, the meaning of the transition density obtained here? What qualitative arguments can be advanced to show that $\rho_o(\theta)$ should be a decreasing function of temperature? To answer these questions it must be realized that the approximations used in the Green functions equations are only valid for $\theta \ll \rho U_o$, and these approximations limited the set of coupled Green functions equations to a pair. As it was shown at the end of Chapter V, this termination of the equations imply that only an instability of the solid-superfluid type can occur in the one-particle Green function. Now regardless of the Green functions obtained from the approximated equations, i.e. regardless of the excitation spectrum that one obtains for the system under consideration, one should obtain that the probability of finding the system in the ground state at sufficiently high temperatures is negligible, that is, one should not find the system in the superfluid state at very high temperatures. Therefore, one should expect to obtain a $\rho_o(\theta)$ which decreases as θ increases and intercepts the $\rho(p=0)$

at a certain value of θ . Had the approximations been much better such as to allow for the possibility of a solid-non superfluid transition in the system, one could have expected $\rho_0(\theta)$ to increase with θ up to $\theta = \theta_\lambda$ at which temperature the character of the transition should change to a solid-normal liquid type of transition.

CHAPTER VII

CONCLUSIONS

A system of non-relativistic Bosons with short range repulsive interactions and nearest neighbor attractive interactions was treated in the quantum cell model. It was found that the density of the solid-superfluid transition did not depend on the strength of the attractive interaction, but only on the mass of the particles and the strength of the repulsive interactions. The density at which the system reaches zero pressure increases as the strength of the attractive interaction increases. Thus it was found that if the strength of the repulsive interaction is large enough, the mass large enough, and the strength of the attractive interaction large enough the transition is inhibited. The exact relations for this condition was found.

A system of non-relativistic Fermions with short range repulsive interactions was treated in the framework of the cell model at $T = 0$. It was shown that the system does not undergo a solid-superfluid transition under any conditions. It was also found that this system has all the particle spins antialigned in the solid state, and that the magnetic field needed to align the spins is too strong to be realizable in the laboratory.

A system of non-relativistic Bosons with short range repulsive interactions at $T \neq 0$ was treated in the framework of the cell model. The specific heat of this system in its solid state was found. It is

typical of a system with a gap in the energy spectrum. The solid-superfluid transition curve for the density versus temperature was obtained. The curve obtained is peculiar to the approximations performed in the solution of the problem and not to be taken seriously.

APPENDICES

APPENDIX A

The following commutators will be obtained in terms of $b_{r_j}(t)$ and $b_{r_j}^*(\tau)$ in this appendix:

$$[b_{r_j}, H]_-, [b_{r_j}^* b_{r_j} b_{r_j}, H]_-, [b_{r_j+r_0}^* b_{r_j+r_0} b_{r_j}, H]_-$$

where H is given by equation (3.1)

First, $[b_{r_j}, H]$ will be obtained:

$$\begin{aligned} [b_{r_j}, b_{r_k}^* b_{r_k}] &= b_{r_j} b_{r_k}^* b_{r_k} - b_{r_k}^* b_{r_k} b_{r_j} \\ &= b_{r_k}^* b_{r_j} b_{r_k} + \delta_{r_j r_k} b_{r_k} - b_{r_k}^* b_{r_k} b_{r_j} \\ &= \delta_{r_j r_k} b_{r_k} \end{aligned} \quad (A.1)$$

$$\begin{aligned} [b_{r_j}, b_{r_k+r_0}^* b_{r_k+r_0}]_- &= b_{r_j} b_{r_k+r_0}^* b_{r_k+r_0} - b_{r_k+r_0}^* b_{r_k+r_0} b_{r_j} \\ &= b_{r_k+r_0}^* b_{r_j} b_{r_k+r_0} + \delta_{r_j r_k} b_{r_k+r_0} - b_{r_k+r_0}^* b_{r_k+r_0} b_{r_j} \\ &= \delta_{r_j r_k} b_{r_k+r_0} \end{aligned} \quad (A.2)$$

$$\begin{aligned} [b_{r_j}, b_{r_k}^* b_{r_k}^* b_{r_k} b_{r_k}]_- &= b_{r_j} b_{r_k}^* b_{r_k}^* b_{r_k} b_{r_k} - b_{r_k}^* b_{r_k}^* b_{r_k} b_{r_k} b_{r_j} \\ &= \delta_{r_j r_k} b_{r_k}^* b_{r_k}^* b_{r_k} + b_{r_k}^* b_{r_j} b_{r_k}^* b_{r_k} b_{r_k} - b_{r_k}^* b_{r_k}^* b_{r_k} b_{r_k} b_{r_j} \\ &= \delta_{r_j r_k} 2 b_{r_k}^* b_{r_k}^* b_{r_k} + b_{r_k}^* b_{r_k}^* b_{r_j} b_{r_k} b_{r_k} - b_{r_k}^* b_{r_k}^* b_{r_k} b_{r_k} b_{r_j} \\ &= 2 \delta_{r_j r_k} b_{r_k}^* b_{r_k}^* b_{r_k} \end{aligned} \quad (A.3)$$

$$\begin{aligned}
[b_{r_j}, b_{r_k}^* b_{r_k} b_{r_k+r_0}^* b_{r_k+r_0}]_- &= b_{r_j} b_{r_k}^* b_{r_k} b_{r_k+r_0}^* b_{r_k+r_0} - b_{r_k}^* b_{r_k} b_{r_k+r_0}^* b_{r_k+r_0} b_{r_j} \\
&= \delta_{r_j r_k} b_{r_k} b_{r_k+r_0}^* b_{r_k+r_0} + b_{r_k}^* b_{r_j} b_{r_k} b_{r_k+r_0}^* b_{r_k+r_0} - \\
&\quad - b_{r_k}^* b_{r_k} b_{r_k+r_0}^* b_{r_k+r_0} b_{r_j} \\
&= 2\delta_{r_j r_k} b_{r_k} b_{r_k+r_0}^* b_{r_k+r_0} + b_{r_k}^* b_{r_k} b_{r_k+r_0}^* b_{r_j} b_{r_k+r_0} - \\
&\quad - b_{r_k}^* b_{r_k} b_{r_k+r_0}^* b_{r_k+r_0} b_{r_j} \\
&= 2\delta_{r_j r_k} b_{r_k} b_{r_k+r_0}^* b_{r_k+r_0} \tag{A.4}
\end{aligned}$$

Collecting these expressions:

$$\begin{aligned}
[b_{r_j}, H]_- &= 6K \sum_{r_k} \delta_{r_j r_k} b_{r_k} - K \sum_{r_k, r_j} \delta_{r_j r_k} b_{r_k+r_0}^+ \\
&\quad + \frac{1}{2} \rho U_0 \sum_{r_k} \delta_{r_j r_k} b_{r_k}^* b_{r_k} b_{r_k} + \\
&\quad + \frac{1}{2} \rho \tilde{U} \sum_{r_k} \delta_{r_j r_k} b_{r_k} b_{r_k+r_0}^* b_{r_k+r_0} \tag{A.6}
\end{aligned}$$

The commutator $[b_{r_j}^* b_{r_j} b_{r_j}, H]$ will be obtained next:

$$\begin{aligned}
\sum_m [b_{r_j}^* b_{r_j} b_{r_j}, b_{r_m}^* b_{r_m}]_- &= \sum_m b_{r_j}^* b_{r_j} b_{r_j} b_{r_m}^* b_{r_m} - b_{r_m}^* b_{r_m} b_{r_j}^* b_{r_j} b_{r_j} \\
&= \sum_{r_m} [b_{r_j}^* b_{r_j} (\delta_{r_j r_m} + b_{r_m}^* b_{r_j}) b_{r_m} - b_{r_m}^* b_{r_m} b_{r_j}^* b_{r_j} b_{r_j}] \\
&= \sum_{r_m} [b_{r_j}^* b_{r_j} \delta_{r_j r_m} b_{r_m} + b_{r_j}^* (\delta_{r_j r_m} + b_{r_m}^* b_{r_j}) b_{r_j} b_{r_m} - b_{r_m}^* b_{r_m} b_{r_j}^* b_{r_j} b_{r_j}]
\end{aligned}$$

$$\begin{aligned}
&= \sum_{r_m} \left\{ 2\delta_{r_j r_m} b_{r_j}^* b_{r_j} b_{r_m} - b_{r_m}^* (\delta_{r_j r_m} b_{r_m} b_{r_j}^*) b_{r_j} b_{r_m} - b_{r_m}^* b_{r_m} b_{r_j}^* b_{r_j} b_{r_m} \right\} \\
&= b_{r_j}^* b_{r_j} b_{r_j} \quad (A.7)
\end{aligned}$$

$$\begin{aligned}
\sum_{m, r_o} [b_{r_j}^* b_{r_j} b_{r_j}, b_{r_m}^* b_{r_m+r_o}] &= \sum_{r_m, r_o} b_{r_j}^* b_{r_j} b_{r_m+r_o} \delta_{r_j r_m} \\
&+ \sum_{r_m, r_o} b_{r_j}^* b_{r_m+r_o} b_{r_j} \delta_{r_m, r_j} - \sum_{r_m, r_o} b_{r_m}^* b_{r_j} b_{r_j} \delta_{r_j, r_m+r_o} \\
&= 2b_{r_j}^* b_{r_j} b_{r_m+r_o} - b_{r_j+r_o}^* b_{r_j} b_{r_j} \quad (A.8)
\end{aligned}$$

$$\begin{aligned}
\sum_{r_m} [b_{r_j}^* b_{r_j} b_{r_j}, b_m^* b_m^* b_m]_- &= \sum_{r_m} \{ b_{r_j}^* b_{r_j} b_{r_m} b_{r_m} b_{r_m} \delta_{r_j, r_m} + \\
&+ b_{r_j}^* b_{r_j} b_{r_m}^* b_{r_m} b_{r_m} \delta_{r_j, r_m} + b_{r_j}^* b_{r_m}^* b_{r_m} b_{r_m} b_{r_j} \delta_{r_j, r_m} + \\
&+ b_{r_j}^* b_{r_m}^* b_{r_m} b_{r_m} b_{r_j} \delta_{r_j r_m} b_{r_m}^* b_{r_m}^* b_{r_m} b_{r_j} \delta_{r_j r_m} - b_{r_m}^* b_{r_m}^* b_{r_m} b_{r_j} b_{r_j} \delta_{r_m, r_j} \} \quad (A.9) \\
&= \sum_{r_m, r_o} [b_{r_j}^* b_{r_j} b_{r_j}, b_{r_m}^* b_{r_m} b_{r_m+r_o}^* b_{r_m+r_o}]_- = \sum_{r_m, r_o} b_{r_j}^* b_{r_j} b_{r_m+r_o}^* b_{r_m+r_o} \delta_{r_j r_m} \\
&+ b_{r_j}^* b_{r_j} b_{r_m}^* b_{r_m} b_{r_m+r_o} \delta_{r_j, r_m+r_o} + b_{r_j}^* b_{r_m} b_{r_m}^* b_{r_m+r_o} b_{r_j} \delta_{r_j, r_m} \\
&+ b_{r_j}^* b_{r_m}^* b_{r_m} b_{r_m+r_o} b_{r_j} \delta_{r_j, r_m+r_o} b_{r_m}^* b_{r_m}^* b_{r_m+r_o} b_{r_m+r_o} b_{r_j} b_{r_j} \delta_{r_j, r_m} \\
&- b_{r_m}^* b_{r_m} b_{r_m+r_o}^* b_{r_j} b_{r_j} \delta_{r_j, r_m+r_o} \\
&= \sum_{r_o} 2b_{r_j}^* b_{r_j} b_{r_j} b_{r_j+r_o}^* b_{r_j+r_o} \quad (A.10)
\end{aligned}$$

Collecting these results one obtains:

$$\begin{aligned}
 [b_{r_j}^* b_{r_j} b_{r_j}, H]_- &= 6K b_{r_j}^* b_{r_j} b_{r_j} - 2K \sum_{r_0} b_{r_j}^* b_{r_j} b_{r_j+r_0} + \\
 &+ K \sum_{r_0} b_{r_j+r_0}^* b_{r_j} b_{r_j} + \rho U_0 b_{r_j}^* b_{r_j} b_{r_j} + \rho U_0 b_{r_j}^* b_{r_j}^* b_{r_j} b_{r_j} + \\
 &+ \sum_{r_0} \rho \tilde{U} b_{r_j}^* b_{r_j} b_{r_j} b_{r_j+r_0}^* b_{r_j+r_0} \quad (A.11)
 \end{aligned}$$

It is also necessary to obtain:

$$\begin{aligned}
 [b_{r_j+r_0}^* b_{r_j+r_0} b_{r_j}, H]_- \\
 \sum_{r_m} [b_{r_j+r_0} b_{r_j+r_0} b_{r_j}, b_{r_m}^* b_{r_m}]_- &= \sum_{r_m} (b_{r_j+r_0}^* b_{r_j+r_0} b_{r_m} \delta_{r_j, r_m} + \\
 &+ b_{r_j+r_0}^* b_{r_m} b_{r_j} \delta_{r_m, r_j+r_0} - b_{r_m}^* b_{r_j+r_0} b_{r_j} \delta_{r_m, r_j+r_0}) \\
 &= b_{r_j+r_0}^* b_{r_j+r_0} b_{r_j} \quad (A.12)
 \end{aligned}$$

$$\begin{aligned}
 \sum_{r_m, r'} [b_{r_j+r_0}^* b_{r_j+r_0} b_{r_j}, b_{r_m}^* b_{r_m+r'}]_- &= \sum_{r_m, r'} (b_{r_j+r_0}^* b_{r_j+r_0} b_{r_m+r'} \delta_{r_j, r_m} + \\
 &+ b_{r_j+r_0}^* b_{r_m+r'} b_{r_j} \delta_{r_m, r_j+r_0} - b_{r_m}^* b_{r_j+r_0} b_{r_j} \delta_{r_m+r', r_j+r_0}) \\
 &= \sum_{r'} (b_{r_j+r_0}^* b_{r_j+r_0} b_{r_j+r'} + b_{r_j+r_0}^* b_{r_j+r_0+r'} b_{r_j} \\
 &\quad - b_{r_j+r_0+r'}^* b_{r_j+r_0} b_{r_j}) \quad (A.13)
 \end{aligned}$$

$$\begin{aligned}
\sum_m [b_{r_j+r_0}^* b_{r_j+r_0} b_{r_j}, b_{r_m}^* b_{r_m}^* b_{r_m} b_{r_m}] &= \sum_m (b_{r_j+r_0}^* b_{r_j+r_0} b_{r_m}^* b_{r_m} b_{r_m} \delta_{r_j, r_m} + \\
&+ b_{r_j+r_0}^* b_{r_j+r_0} b_{r_m}^* b_{r_m} b_{r_m} \delta_{r_j, r_m} + 2b_{r_j+r_0}^* b_{r_m}^* b_{r_m} b_{r_m} b_{r_j} \delta_{r_j+r_0, r_m} + \\
&- 2b_{r_m}^* b_{r_m}^* b_{r_m} b_{r_j+r_0} b_{r_j} \delta_{r_m, r_j+r_0}) \\
&= 2b_{r_j+r_0}^* b_{r_j+r_0} b_{r_j}^* b_{r_j} b_{r_j} \quad (A.14)
\end{aligned}$$

$$\begin{aligned}
\sum_{r_m, r'} b_{r_j+r_0}^* b_{r_j+r_0} b_{r_j}, b_{r_m}^* b_{r_m}^* b_{r_m+r'} b_{r_m+r'} &= \\
&= \sum_{r_m, r'} b_{r_j+r_0}^* b_{r_j+r_0} b_{r_m}^* b_{r_m+r'} b_{r_m+r'} \delta_{r_j, r_m} + \\
&+ b_{r_j+r_0}^* b_{r_j+r_0} b_{r_m}^* b_{r_m} b_{r_m+r'} \delta_{r_j, r_m+r'} + \\
&+ b_{r_j+r_0}^* b_{r_m} b_{r_m+r'}^* b_{r_m+r'} b_{r_j} \delta_{r_m, r_j+r_0} + \\
&+ b_{r_j+r_0}^* b_{r_m}^* b_{r_m} b_{r_m+r'} b_{r_j} \delta_{r_j+r_0, r_m+r'} + \\
&- b_{r_m}^* b_{r_m+r'}^* b_{r_m+r'} b_{r_j+r_0} b_{r_j} \delta_{r_j+r_0, r_m} - \\
&- b_{r_m}^* b_{r_m} b_{r_m+r'}^* b_{r_j+r_0} b_{r_j} \delta_{r_j+r_0, r_m+r'} \\
&= \sum_{r'} b_{r_j+r_0}^* b_{r_j+r_0} b_{r_j} b_{r_j+r'}^* b_{r_j+r'} + b_{r_j+r_0}^* b_{r_j+r_0} b_{r_j+r'}^* b_{r_j+r'} b_{r_j} + \\
&+ b_{r_j+r_0}^* b_{r_j+r_0} b_{r_j+r_0+r'}^* b_{r_j+r_0+r'} b_{r_j} + b_{r_j+r_0}^* b_{r_j+r_0+r'}^* b_{r_j+r'} b_{r_j+r_0} b_{r_j} \\
&- b_{r_j+r_0}^* b_{r_j+r_0+r'}^* b_{r_j+r_0+r'} b_{r_j+r_0} b_{r_j} - b_{r_j+r_0+r'}^* b_{r_j+r_0+r'} b_{r_j+r_0}^* b_{r_j+r_0} b_{r_j} \\
&= \sum_{r'} 2b_{r_j+r_0}^* b_{r_j+r_0} b_{r_j+r'}^* b_{r_j+r'} b_{r_j} \quad (A.15)
\end{aligned}$$

Therefore

$$\begin{aligned}
 [b_{r_j+r_o}^* b_{r_j+r_o} b_{r_j}, H]_- &= 6K b_{r_j+r_o}^* b_{r_j+r_o} b_{r_j} - \\
 &- K \sum_{r'} (b_{r_j+r_o}^* b_{r_j+r_o} b_{r_j+r'} + b_{r_j+r_o}^* b_{r_j+r_o+r'} b_{r_j} - \\
 &- b_{r_j+r_o+r'}^* b_{r_j+r_o} b_{r_j}) + \rho U_o b_{r_j+r_o}^* b_{r_j+r_o} b_{r_j}^* b_{r_j} b_{r_j} - \\
 &+ \rho U \sum_{r'} b_{r_j+r_o}^* b_{r_j+r_o} b_{r_j+r'}^* b_{r_j+r'} b_{r_j} \quad (A.16)
 \end{aligned}$$

APPENDIX B

The value of $h = \sum_{\mathbf{r}'} \langle \varphi_0 | b_{\mathbf{r}_j}^* b_{\mathbf{r}_j + \mathbf{r}'} | \varphi_0 \rangle$ will be obtained in this appendix, within the approximations of Chapter III. From equation (3.31) and (3.32)

$$G_1(k, \omega) = \frac{\omega - 6K - 6\rho\tilde{U} + \rho U_0}{\omega_+ - \omega_-} \frac{1}{\omega - \omega_+} - \frac{1}{\omega - \omega_-} \quad (\text{B.1})$$

$$\begin{aligned} \omega_{\pm} = 6K + \frac{\rho U_0}{2} - \frac{k}{2} \sum_{\mathbf{r}'} e^{i\bar{\mathbf{k}} \cdot \bar{\mathbf{r}}'} + 6\rho\tilde{U} \pm \\ \pm \sqrt{\left(\frac{\rho U_0}{2} - \frac{k}{2} \sum_{\mathbf{r}'} e^{i\bar{\mathbf{k}} \cdot \bar{\mathbf{r}}'}\right)^2 - \rho U_0 K \sum_{\mathbf{r}'} e^{i\bar{\mathbf{k}} \cdot \bar{\mathbf{r}}'} + \rho U_0 K h} \end{aligned} \quad (\text{B.2})$$

Now

$$h = \frac{i}{(2\pi)^4} (r_0)^3 \int G(k, \omega) \sum_{\mathbf{r}'} e^{i\bar{\mathbf{k}} \cdot \bar{\mathbf{r}}'} e^{-i\omega_0^-} d^3k d\omega \quad (\text{B.3})$$

After integrating with respect to ω , the previous equation reads:

$$h = \frac{(r_0)^3}{(2\pi)^3} \sum_{\mathbf{r}'} \int e^{i\bar{\mathbf{k}} \cdot \bar{\mathbf{r}}'} \left(-\frac{1}{2} + \frac{\frac{3\rho U_0}{2} - \frac{K}{2} \sum_{\mathbf{r}'} e^{i\bar{\mathbf{k}} \cdot \bar{\mathbf{r}}'}}{\omega_+ - \omega_-} \right) d^3k$$

This integral has been evaluated in effect in Gersch²⁵ and Knollman's paper. The result is

$$h = 12x$$

to first order in x .

APPENDIX C

The value of $h = \sum_{\mathbf{r}'} \varphi_0 |b_{\mathbf{r}_j}^* b_{\mathbf{r}_j + \mathbf{r}'}| \varphi_0$ will be obtained in this appendix, within the approximations of Chapter IV.

Let

$$G_1(j, k; t) = \sum_{n=0}^{\infty} K^n G_1^{(n)}(j, k; t) \quad (\text{C.1})$$

Substituting this expression into equation (4.16) one obtains after some simplification an equation for $G_1^{(0)}$.

$$\begin{aligned} (\omega - 6K - 6\rho\tilde{U})(\omega - 6K - 6\rho\tilde{U} - \rho U_0) G_1^{(0)}(j, k; \omega) = \\ = \delta_{\mathbf{r}_j, \mathbf{r}_k} (\omega - 6K - 6\rho\tilde{U} + \rho U_0) \end{aligned} \quad (\text{C.2})$$

The solution to this equation is:

$$G_1^{(0)}(j, k) = \frac{-1}{\omega - 6K - 6\rho\tilde{U} - i\eta} - \frac{2}{\omega - 6K - 6\rho\tilde{U} - \rho U_0 + i\eta} \delta_{\mathbf{r}_j, \mathbf{r}_k} \quad (\text{C.3})$$

let

$$A(\omega) = - \frac{1}{\omega - 6K - 6\rho\tilde{U} - i\eta} + \frac{2}{\omega - 6K - 6\rho\tilde{U} - \rho U_0 + i\eta} \quad (\text{C.4})$$

$$G_1^{(0)}(j, k; \omega) = \delta_{\mathbf{r}_j, \mathbf{r}_k} A(\omega)$$

The next equation obtained relates $G_1^{(0)}(j, k; \omega)$ and $G_1^{(1)}(j, k; \omega)$.

$$h^{(1)} = \frac{i}{2\pi} \int G_1^{(1)}(r_j + r', r_j; 0) e^{-i\omega_0^-} d\omega \quad (C.9)$$

From (C.6) it follows that:

$$h^{(1)} = \frac{i}{(2\pi)} \int \left[-A^2(\omega) + \frac{2\rho U A(\omega)}{(\omega - 6K - i\eta)(\omega - 6K - 6\rho U - i\eta)} + \right. \\ \left. + \frac{h^{(1)} \rho U}{6(\omega - 6K - i\eta)(\omega + 6K - 6\rho U - i\eta)} \right] e^{-i\omega_0^-} d\omega \quad (C.10)$$

Now

$$- \frac{i}{2\pi} \int A^2(\omega) e^{-i\omega_0^-} d\omega = \frac{24}{\rho U_0} \quad (C.11)$$

and

$$\frac{i}{2\pi} \int \frac{2\rho U A(\omega) e^{-i\omega_0^-}}{(\omega - 6K - i\eta)(\omega - 6K - 6\rho \tilde{U} - i\eta)} d\omega = \\ = \frac{i}{2\pi} \int 2\rho \tilde{U} \left[- \frac{1}{(\omega - 6K - 6\rho \tilde{U} - i\eta)^2 (\omega - 6K - i\eta)} + \right. \\ \left. + \frac{2}{(\omega - 6K - i\eta)(\omega - 6K - 6\rho \tilde{U} - i\eta)(\omega - 6K - 6\rho \tilde{U} - \rho U_0 + i\eta)} \right] e^{-i\omega_0^-} d\omega \\ = \frac{i}{2\pi} \int \frac{2\rho \tilde{U}}{6\rho \tilde{U}} \frac{1}{6\rho U} \frac{1}{(\omega - 6K - 6\rho \tilde{U} - i\eta)} - \frac{1}{6\rho \tilde{U}} \frac{1}{(\omega - 6K - i\eta)} - \\ - \frac{1}{(\omega - 6K - 6\rho \tilde{U} - i\eta)^2} + \\ \left. + \frac{12\rho U}{(\omega - 6K - i\eta)(\omega - 6K - 6\rho \tilde{U} - i\eta)(\omega - 6K - 6\rho U - \rho \tilde{U}_0 + i\eta)} \right] e^{-i\omega_0^-} d\omega \quad (C.13)$$

The previous expression equals:

$$\frac{i}{2\pi} 2\pi i \left[\frac{1}{6\rho\tilde{U}} - \frac{1}{6\rho\tilde{U}} - \frac{12\rho\tilde{U}}{6\rho\tilde{U}\rho U_0} + \frac{12\rho\tilde{U}}{6\rho\tilde{U}(\rho U_0 + 6\rho U)} \right] \simeq 12 \frac{\rho U}{(\rho\tilde{U}_0)^2}$$

Also

$$\int \frac{h^{(1)}}{6} \frac{\rho\tilde{U}}{(\omega - 6K - i\eta)(\omega - 6K - 6\rho\tilde{U} - i\eta)} e^{-i\omega b^-} d\omega = 0 \quad (C.14)$$

therefore

$$h^{(1)} = 12 \frac{2}{\rho U_0} + 12 \frac{2\rho\tilde{U}}{(\rho U_0)^2}$$

$$\text{but } h = h^{(0)} + kh^{(1)} + \dots$$

So

$$h = 12x (1 + y)$$

$$\text{where } y = \frac{\rho\tilde{U}}{\rho U_0}, \text{ to first power in } x.$$

APPENDIX D

The commutator $[b_{\sigma r_j}, H]_-$ will be obtained in this appendix.

H is the Hamiltonian for a system of Fermions.

$$\begin{aligned}
 H = & 6K \sum_{r_j, \sigma} b_{\sigma r_j}^* b_{\sigma r_j} - K \sum_{\sigma r_j, r'} b_{\sigma r_j}^* b_{\sigma r_j + r'} + \\
 & + \frac{1}{2} \rho U_0 \sum_{\sigma \sigma' r_j} b_{\sigma r_j}^* b_{\sigma' r_j}^* b_{\sigma' r_j} b_{\sigma r_j}
 \end{aligned} \quad (D.1)$$

and the operators $b_{\sigma r_j}$ satisfy the relations:

$$\begin{aligned}
 [b_{\sigma r_j}, b_{\sigma' r_k}^*]_+ &= \delta_{\sigma \sigma'} \delta_{r_j, r_k} \\
 [b_{\sigma r_j}, b_{\sigma' r_k}]_+ &= 0. \\
 \sum_{r_k \sigma'} [b_{\sigma r_j}, b_{\sigma' r_k}^* b_{\sigma' r_k}]_- &= \sum_{\sigma r_k} \delta_{\sigma \sigma'} \delta_{r_j r_k} b_{\sigma' r_k} \\
 &= b_{\sigma r_j}
 \end{aligned} \quad (D.2)$$

$$\begin{aligned}
 \sum_{r_k, r', \sigma'} [b_{\sigma r_j}, b_{\sigma' r_k}^* b_{\sigma' r_k + r'}]_- &= \sum_{r_k, r', \sigma'} \delta_{r_j r_k} \delta_{\sigma \sigma'} b_{r_k + r', \sigma'} \\
 &= b_{r_j + r', \sigma}
 \end{aligned} \quad (D.3)$$

$$\begin{aligned}
 \sum_{r_k, \sigma'', \sigma'} [b_{\sigma r_j}, b_{\sigma' r_k}^* b_{\sigma'' r_k}^* b_{\sigma'' r_k} b_{\sigma' r_k}]_- &= \sum_{r_k, \sigma', \sigma''} (\delta_{r_j r_k} \delta_{\sigma \sigma'} b_{r_k \sigma''}^* b_{r_k \sigma''} b_{r_k \sigma''} b_{r_k \sigma'} - \\
 &- b_{\sigma' r_k}^* b_{\sigma'' r_k} b_{\sigma'' r_k} b_{\sigma' r_k} \delta_{r_j r_k} \delta_{\sigma'' \sigma})
 \end{aligned} \quad (D.4)$$

Therefore

$$[b_{\sigma r_j}, H]_- = 6K b_{\sigma r_j} - K \sum_{r'} b_{\sigma r_j+r'} + \rho U_0 b_{\sigma', r_j}^* b_{\sigma', r_j} b_{\sigma r_j}$$

It is also necessary to obtain an expression for $[b_{\sigma', r_j}^* b_{\sigma', r_j} b_{\sigma r_j}, H]_-$ to obtain the equation of motion to $G_2(j, \sigma', j\sigma; t)_-$

$$\begin{aligned} \sum_{r_k \sigma''} [b_{\sigma', r_j}^* b_{\sigma', r_j} b_{\sigma r_j}, b_{r_k \sigma''}^* b_{r_k \sigma''}]_- &= \sum_{r_k \sigma''} (b_{\sigma', r_j}^* b_{\sigma', r_j} b_{\sigma''} r_k \delta_{r_j r_k} \delta_{\sigma \sigma''} + \\ &+ b_{\sigma', r_j}^* b_{\sigma''} r_k b_{\sigma r_j} \delta_{r_j r_k} \delta_{\sigma \sigma''} - b_{\sigma''} r_k b_{\sigma', r_j} b_{\sigma r_j} \delta_{r_j r_k} \delta_{\sigma', \sigma''}) \\ &= b_{\sigma', r_j}^* b_{\sigma', r_j} b_{\sigma r_j} \end{aligned} \quad (D.6)$$

$$\begin{aligned} \sum_{r_k, \sigma'', r'} [b_{\sigma', r_j}^* b_{\sigma', r_j} b_{\sigma r_j}, b_{\sigma''}^* r_k b_{\sigma''} r_{k+r'}]_- &= \\ &= \sum_{\sigma'', r_k, r'} (b_{\sigma', r_j}^* b_{\sigma', r_j} b_{\sigma''} r_{k+r'} \delta_{r_j r_k} \delta_{\sigma \sigma''} + \\ &+ b_{\sigma', r_j}^* b_{\sigma''} r_{k+r'} b_{\sigma r_j} \delta_{r_j r_k} \delta_{\sigma', \sigma''} - b_{\sigma''}^* r_k b_{\sigma', r_j} b_{\sigma r_j} \delta_{r_j, r_{k+r'}} \delta_{\sigma', \sigma''}) \\ &= \sum_{r'} (b_{\sigma', r_j}^* b_{\sigma', r_j} b_{\sigma r_{j+r'}} + b_{\sigma', r_j}^* b_{\sigma', r_{j+r'}} b_{\sigma r_j} - \\ &\quad - b_{\sigma', r_{j+r'}}^* b_{\sigma', r_j} b_{\sigma r_j}) \quad (D.7) \end{aligned}$$

$$\begin{aligned}
& \sum_{r_k, \sigma'', \sigma'''} [b_{\sigma', r_j}^* b_{\sigma', r_j} b_{\sigma, r_j} b_{\sigma'', r_k} b_{\sigma'', r_k} b_{\sigma'', r_k} b_{\sigma'', r_k}]_- = \\
& = \sum_{r_k, \sigma'', \sigma'''} (b_{\sigma', r_j}^* b_{\sigma', r_j} b_{\sigma'', r_k}^* b_{\sigma'', r_k} b_{\sigma'', r_k} \delta_{r_j r_k} \delta_{\sigma \sigma'' \sigma'''} - \\
& - b_{\sigma', r_j}^* b_{\sigma', r_j} b_{\sigma'', r_k}^* b_{\sigma'', r_k} b_{\sigma'', r_k} \delta_{r_j r_k} \delta_{\sigma \sigma''} + \\
& + b_{\sigma', r_j}^* b_{\sigma'', r_k}^* b_{\sigma'', r_k} b_{\sigma'', r_k} \delta_{r_j r_k} \delta_{\sigma', \sigma'' \sigma'''} b_{\sigma, r_j} - \\
& - b_{\sigma', r_j}^* b_{\sigma'', r_k}^* b_{\sigma'', r_k} b_{\sigma'', r_k} b_{\sigma, r_j} \delta_{r_j r_k} \delta_{\sigma', \sigma''} + \\
& + b_{\sigma'', r_k}^* b_{\sigma'', r_k}^* b_{\sigma'', r_k} b_{\sigma', r_j} b_{\sigma', r_j} b_{\sigma, r_j} \delta_{r_j r_k} \delta_{\sigma', \sigma'''} \\
& - b_{\sigma'', r_k}^* b_{\sigma'', r_k}^* b_{\sigma'', r_k} b_{\sigma', r_j} b_{\sigma, r_j} \delta_{r_j r_k} \delta_{\sigma', \sigma'' \sigma'''}) \\
& = b_{\sigma', j}^* b_{\sigma', j} b_{\sigma', j}^* b_{\sigma', j} b_{\sigma, j} - b_{\sigma', j}^* b_{\sigma', j} b_{\sigma', j}^* b_{\sigma, j} b_{\sigma', j} + b_{\sigma', j}^* b_{\sigma', j} b_{\sigma, j} b_{\sigma', j}^* b_{\sigma, j} - \\
& - b_{\sigma', j}^* b_{\sigma', j} b_{\sigma', j}^* b_{\sigma, j} b_{\sigma, j} + b_{\sigma', j}^* b_{\sigma', j} b_{\sigma, j} b_{\sigma', j}^* b_{\sigma, j} - b_{\sigma', j}^* b_{\sigma', j} b_{\sigma, j} b_{\sigma', j}^* b_{\sigma, j} \\
& = 2b_{\sigma', j}^* b_{\sigma', j} b_{\sigma', j}^* b_{\sigma', j} b_{\sigma', j} b_{\sigma, j} \\
& = b_{\sigma', j}^* b_{\sigma', j} b_{\sigma, j} \tag{D.8}
\end{aligned}$$

therefore

$$\begin{aligned}
[b_{\sigma', j}^* b_{\sigma'', j} b_{\sigma, r_j}, H]_- &= 6K b_{\sigma', r_j}^* b_{\sigma', r_j} b_{\sigma, r_j} - K \sum_{r'} b_{\sigma', r_j} b_{\sigma', r_j} b_{r_j + r', \sigma} - \\
& - K \sum_{r'} b_{\sigma', r_j} b_{\sigma', r_j + r'} b_{\sigma, r_j} + K \sum_{r'} b_{\sigma', r_j + r'} b_{\sigma', r_j} b_{\sigma, r_j} \\
& + \rho U_0 b_{\sigma', r_j}^* b_{\sigma', r_j} b_{\sigma, r_j} \tag{D.9}
\end{aligned}$$

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